

Institute of Electrical and Electronics Engineers  
IEEE Nanotechnology Council  
Montenegrin Science Promotion Foundation  
Sumy State University

**2026 IEEE 16<sup>th</sup> International Conference  
“Nanomaterials: Applications &  
Properties” (IEEE NAP-2026)**

**NAN  materials:  
Applications &  
Properties -2026**

**BOOK OF ABSTRACTS**



*Budva, Montenegro  
2026*

## Welcome Message

---

*Dear Colleagues,*

*It is our pleasure to welcome you to the 2026 IEEE 16th International Conference on Nanomaterials: Applications and Properties (IEEE NAP-2026), held from 6 to 11 September 2026 at the Avala Resort in Budva, on the Adriatic coast of Montenegro.*

*For sixteen years, NAP has brought together the people who move nanoscience forward: physicists, chemists, materials scientists, engineers, and the students who will carry the field into its next decade. The work collected in this book spans twelve tracks and is anchored by four plenary lectures. It brings together 78 invited talks, 70 oral and 131 poster presentations (including 58 remote e-Posters), contributed by researchers from 41 countries. Following NAP tradition, every submitted manuscript undergoes rigorous peer review, and accepted papers will be proposed for inclusion in the IEEE Xplore Digital Library and additional indexing databases.*

*Beyond the talks and posters, we hope you find time for Budva itself: its walled old town, the Adriatic, and the unhurried company of colleagues old and new.*

*Welcome to Montenegro, and welcome to NAP-2026.*

*With warm regards,*

*Goran Karapetrov and Valentine Novosad  
General Chairs, IEEE NAP-2026*

---

## IEEE NAP-2026 Sponsors

---



The **IEEE Nanotechnology Council** is a multidisciplinary group advancing the theory, design, and development of nanotechnology and its scientific, engineering, and industrial applications. It sponsors well-recognized international conferences and publications, and through its activities participants publish and collaborate on research, network with colleagues, stay current on news and events, develop standards, and take part in educational programs. There are no membership requirements to join, and participation is free for current IEEE members.



The **Montenegrin Science Promotion Foundation (PRONa)** is a national nonprofit organization dedicated to advancing scientific research, education, and innovation in Montenegro. It supports initiatives that strengthen international collaboration, promote excellence in STEM disciplines, and foster engagement between academia, industry, and society. Through conferences, educational programs, and outreach, the Foundation helps build a vibrant and globally connected scientific community.



**Sumy State University (SumDU)** holds a special place in the life of this conference: it is where IEEE NAP was born, in 2011, and from which the series has grown into the international meeting we gather for today, now in its 16th edition. One of Ukraine's leading public research universities, based in the city of Sumy, SumDU has developed a strongly international character, welcoming students and scholars from around the world and sustaining academic partnerships across nearly fifty countries. Its teaching reaches across the natural and engineering sciences, medicine, and the humanities, and is matched by a vibrant research culture; the university is recognized in the QS World University Rankings for its research intensity. Through times of real adversity, SumDU has continued to teach, to discover, and to look outward to the global academic community, and it remains a proud co-organizer of the IEEE NAP Conference.

## Organizing Committee

---

<b>Goran Karapetrov</b>	General Chair - Drexel University, USA
<b>Valentine Novosad</b>	General Chair - Argonne National Laboratory, USA
<b>Alexander Pogrebnyak</b>	General Co-Chair - Sumy State University, Ukraine; Slovak University of Technology in Bratislava, Slovakia
<b>Jovan Mirković</b>	Local Organizing Committee Chair - Montenegrin Science Promotion Foundation, Montenegro
<b>Yurii Shabelnyk</b>	Secretary - Sumy State University, Ukraine
<b>Oleksandr Prokopenko</b>	Publication Chair - Taras Shevchenko National University of Kyiv, Ukraine
<b>Nikša Bulatović</b>	Finance Chair - Montenegrin Science Promotion Foundation, Montenegro
<b>Andrii Chumak</b>	Awards & Grants Chair - University of Vienna, Austria
<b>Anna Nenia</b>	WiSE Chair - Sumy State University
<b>Marian Precner</b>	IT & Technical Support Chair - Institute of Electrical Engineering, SAS, Slovakia
<b>Matteo Bruno Lodi</b>	YP & Students Activities Chair - University of Cagliari, Italy

## Conference Program Committee

---

<b>Goran Karapetrov</b>	Chair - Drexel University, USA
<b>Andrii Chumak</b>	University of Vienna, Austria
<b>Milan Ćapajna</b>	Institute of Electrical Engineering, SAS, Slovakia
<b>Vladimír Cambel</b>	Institute of Electrical Engineering, SAS, Slovakia
<b>Vierka Skakalová</b>	Institute of Electrical Engineering, SAS, Slovakia
<b>Maksym Pogorielov</b>	University of Latvia; Sumy State University

## International Scientific Advisory Board

---

Valentine Novosad (Chair, USA); Maksym Pogorielov (Co-Chair, Latvia/Ukraine); André Anders (Germany); Aleksandra Baron-Wiechec (China); Oksana Chubykalo-Fesenko (Spain); Nicola Pinna (Germany); Kremena Makasheva (France); Denise Erb (Germany); Ali Erdemir (USA); Yury Gogotsi (USA); Laura H. Greene (USA); Vladimir Tsukruk (USA); James E. Morris (USA); Vierka Skakalová (Slovakia); Oleksiy Kolezhuk (Ukraine); Vladimir Komanicky (Slovakia); Oleg Lupan (Moldova); Yuko Ichiyanagi (Japan); Tetsuya Nakamura (Japan); Alexander Pogrebnyak (Ukraine); Sara Majetich (USA); Tijana Rajh (USA); Montserrat Rivas (Spain); Modris Greitāns (Latvia); Oksana Sulaieva (Ukraine); Tetiana Tatarchuk (Ukraine); Oleksandr Tovstolytkin (Ukraine); Nicoletta Ditaranto (Italy).

## Contents

---

Plenary Lectures .....	5
Track 1. Nanomaterials Synthesis and Design.....	10
Track 2. MXenes: Physics, Chemistry, and Applications .....	66
Track 3. Quantum Materials, Devices, and Phenomena .....	78
Track 4. Electrochemistry of Nanomaterials, and Advanced Energy Storage .....	88
Track 5. Multifunctional Thin Films and Advanced Coatings.....	103
Track 6. Ultrawide Bandgap Materials and Nanophotonics .....	141
Track 7. Magnetic Materials, Magnonics and Spin Phenomena.....	150
Track 8. Superconductivity in Nanoscale and Mesoscopic Systems .....	197
Track 9. Nanosensors, Nanodevices and Functional Systems .....	205
Track 10. Nanomaterials for Energy and Environmental Technologies .....	233
Track 11. Nanobiomedical Research and Translational Applications.....	266
Track 12. Enabling Technologies and Emerging Directions.....	291
Author Index.....	301

---

Copyright © 2026 IEEE NAP. All rights reserved.

This Book of Abstracts and its contents are the copyrighted property of the IEEE NAP-2026 conference and the respective authors. No part may be reproduced, redistributed, or stored in a retrieval system without prior written permission. This work is not licensed for use in artificial-intelligence training, text or data mining, or automated scraping.

Individual abstracts remain the intellectual property of their authors and are reproduced here with permission.

# Plenary Lectures

## Composition - structure - property relationships in MXenes

Babak Anasori<sup>1</sup> \*

1) School of Materials Engineering and School of Mechanical Engineering Purdue University, West Lafayette, IN 47907, USA

\* banasori AT purdue.edu

Since their discovery 15 years ago, MXenes, a large family of two-dimensional (2D) transition metal carbides, nitrides, and carbonitrides, have expanded the landscape of nanomaterials science. With over 100 synthesized compositions to date, the rapid growth of the MXene family is driven by designer chemistry control of their composition and structures, including the transition metals, non-metal X sublattice, surface functional groups, and atomic-layer configurations. This large compositional and structural space enables systematic tuning of electronic structure, chemical ordering, defects, surface chemistry, and functional properties. In addition to their chemical and structural diversity, MXenes are known for their high electrical conductivity, hydrophilicity, solution processability, and mechanical robustness, making them attractive for a broad range of applications in nanotechnology.

In this talk, I will discuss how composition and structure govern the properties of MXenes across different length scales. I will present our recent efforts on compositionally complex MXenes, including medium- and high-entropy systems with up to nine transition metals, and discuss how entropy drives transitions from ordered to disordered structures at sub-nanometer thicknesses. I will also discuss how atomic-level defect engineering, including control of vacancies, substitutional defects, and surface chemistry, enables tuning of properties such as electrocatalytic behavior, electrical conductivity, oxidation resistance, and high-temperature stability. Together, these studies demonstrate how compositional and structural control can be used to design MXenes with targeted functionalities.

---

### REFERENCES

- [1] A. Thakur *et al.*, Composition-structure-property relationships in MXenes. *Nature Reviews Materials* (2026)
- [2] B. C. Wyatt *et al.*, Order-to-disorder transition due to entropy in layered and 2D carbides. *Science* 389,1054-1058 (2025)

---

### PLENARY SPEAKER



#### Babak Anasori

Dr. Babak Anasori is the Reilly Rising Star Associate Professor at Purdue University, with joint appointments in the Schools of Materials Engineering and Mechanical Engineering. He also serves as the Editor-in-Chief of *Graphene and 2D Materials*, a Springer-Nature journal. Dr. Anasori received his PhD from Drexel University in 2014 in the Department of Materials Science and Engineering, the birthplace of MXenes. He has authored over 210 refereed publications on MXenes and their precursors and has been a Web of Science Highly Cited Researcher since 2019. His awards include the 2016 MRS Postdoctoral Award, the 2021 Drexel 40-under-40, the 2021 Waterloo Institute for Nanotechnology Rising Star Award, the 2024 ACerS Early Discovery Award, the 2024 Kavli Foundation Early Career Lectureship in Materials Science (MRS), and the 2026 Purdue Faculty Excellence Award for Early Career Research. His lab develops novel 2D carbide and carbonitride MXenes for energy generation, electromagnetic interference shielding, and ultra-high-temperature and extreme environments.

## Tuning perovskite nanoparticles through surface modification

Tijana Rajh<sup>1</sup>\*, Ayendrila Das<sup>1</sup>

1) School of Molecular Sciences, Arizona State University, Tempe AZ 85281, USA

\* Tijana.Rajh AT asu.edu

Perovskite solar cells have emerged as promising candidates for next-generation photovoltaics, demonstrating remarkable advances in both efficiency and cost-effectiveness. Surface modification is a valuable materials engineering strategy employed to address structural imperfections, passivate electronic defects, and align energy levels in perovskite solar cells. This approach becomes even more critical when incorporating perovskite zero-dimensional quantum dots into three-dimensional films, as it helps to heal surface imperfections and improve the overall topography.

Modifiers with specific dipole moments can create hybrid composites in these nanostructured three-dimensional films, combining the electronic properties of semiconductors with the localized characteristics of the organic modifier. This hybridization can tune the work function and establish a smoother energy pathway for electrons or holes to transition into the transporting layers. Applying self-assembled organic molecule monolayers and quantum dots can significantly reduce charge recombination and enhance both efficiency and long-term device stability. Additionally, hydrophobic molecular layers can protect the highly moisture-sensitive perovskite crystal from degradation in ambient conditions.

In our research, we demonstrate that surface modification of perovskite zero-dimensional quantum dots with perylene modifiers can enhance the electron-transfer properties of high-work-function perovskites (FAPbI<sub>3</sub>) towards perylene (N,N'-Bis(2,5-di-tert-butylphenyl)-3,4,9,10-perylene dicarboximide, PDC). This enables perylene to effectively function as an electron-transporting layer, potentially replacing fullerenes as electron carriers in perovskite solar cells. Furthermore, perovskite quantum dots with suitable band gap properties and lower work functions and similar structures (FAPbBr<sub>3</sub>), can undergo energy transfer with the same perylene PDC, making them ideal materials for Perovskite Light-Emitting Diodes (PeLEDs), leading to new technology that has the potential to revolutionize displays and lighting solutions by offering high efficiency, bandwidth, color purity, and low-cost fabrication methods.

---

### PLENARY SPEAKER



#### Tijana Rajh

Tijana Rajh has extensive experience in the synthesis and study of colloidal semiconductor nanocrystals and their integration into hierarchical assembly. She conducted some of the earliest research on quantum dots, a field that has since grown enormously. Her early studies involved electron-transfer reactions and photoelectrochemistry of colloidal semiconductors and quantum dots, solar energy conversion into chemical fuels, and surface modification of nanocrystalline TiO<sub>2</sub> nanoparticles for light-induced chemistries. She developed methods for seamless electronic integration of chelating ligands and colloidal semiconductors, applied magnetic-resonance techniques to study spin effects in photoinduced electron transfer, and proposed early methods to initiate reactions between semiconductor nanoparticles and biomolecules such as DNA strands and antibodies. Her current work focuses on self-adapting nanostructures for energy transduction, conversion and storage, and hybrid systems for sensing of biomolecules, including quantum qubits.

## Structure control of metal clusters and their application in energy and environmental catalysts

Yuichi Negishi<sup>1</sup> \*

<sup>1)</sup> Tohoku University, Japan

\* yuichi.negishi.a8 AT tohoku.ac.jp

In order to build a sustainable society, it is indispensable to create new innovative materials that can solve the problems of the current society. Strict control of the structure of materials at the nanoscale is expected to lead to the creation of such materials. Ultrafine metal clusters, in which several to several dozen metal atoms are aggregated, have novel electronic/geometric structures and physicochemical properties/functions that are different from those of bulk metals composed of the same elements. In addition, doping (alloying) of different elements to these metal clusters results in a variety of structures, properties, and functions. Thus, metal clusters have high potential as constituent units for innovative materials. However, in order to understand the functions of metal clusters and to apply them as materials, it is essential to establish techniques to strictly control the chemical composition and geometric structure of metal clusters. We have established several techniques to strictly control the chemical composition and geometric structure of metal clusters. We also succeeded in establishing a method to control the supported metal clusters to enhance the functionality of advanced water splitting photocatalysts, fuel cell electrocatalysts, and automotive exhaust gas purifying catalysts. Accordingly, we have achieved the highest water-splitting activity for UV-responsive BaLa<sub>4</sub>Ti<sub>4</sub>O<sub>15</sub> water-splitting photocatalysts, created platinum electrocatalysts with higher catalytic activity for oxygen reduction than those currently used in fuel cells, and succeeded in developing highly functional catalysts for automotive exhaust gas purification. These our research is unique in that it consistently achieves the atomic-level control of the metal clusters throughout the entire research, from synthesis to control on the support. This presentation summarizes our recent works concerning these topics[1-5].

**ACKNOWLEDGEMENTS:** This study was supported by the Environment Research and Technology Development Fund (JPMEERF20253003) of the Environmental Restoration and Conservation Agency provided by Ministry of the Environment of Japan, JSPS KAKENHI (grant no. 23H00289 and 23KK0098), Chubu Electric Power Nuclear Safety Research Institute Research Grant, and the FUSO Innovative Technology Fund.

### REFERENCES

- [1] S. Biswas, D.-e. Jiang,\* Y. Negishi\*, *et al.*, "Atomically Precise [Cu<sub>23</sub>H<sub>4</sub>(SC<sub>7</sub>H<sub>7</sub>)<sub>18</sub>(PPh<sub>3</sub>)<sub>6</sub>] Nanocluster: Structural Integration of Johnson Solids through a Cu(0) Center and Electrocatalytic Functionality", *J. Am. Chem. Soc.* 147, 23733–23742, 2025.
- [2] H. Sakai, Y. Negishi,\* T. Hasobe\*, *et al.*, "Bidirectional Intramolecular Singlet and Triplet Energy Transfer in Tetracene-Ultrasmall Gold Nanocluster Dyads: An Evaluation of the Triplet Behavior of Gold Nanoclusters", *J. Am. Chem. Soc.* 147, 13483-13490, 2025.
- [3] M. Sera, S. Hossain,\* Y. Negishi\*, *et al.*, "Atomically Precise Au<sub>24</sub>Pt(thiolate)<sub>12</sub>(dithiolate)<sub>3</sub> Nanoclusters with Excellent Electrocatalytic Hydrogen Evolution Reactivity", *J. Am. Chem. Soc.* 146, 29684–29693, 2024.
- [4] T. Kawawaki, Y. Negishi\*, *et al.*, "Ultrafine Rhodium-Chromium Mixed-Oxide Cocatalyst with Facet-Selective Loading for Excellent Photocatalytic Water Splitting", *J. Am. Chem. Soc.* 146, 26808–26818, 2024.
- [5] S. Biswas, B. Sahoo,\* B. Pathak,\* Y. Negishi\*, *et al.*, "Luminescent Hydride-Free [Cu<sub>7</sub>(SC<sub>5</sub>H<sub>9</sub>)<sub>7</sub>(PPh<sub>3</sub>)<sub>3</sub>] Nanocluster: Facilitating Highly Selective C-C Bond Formation", *J. Am. Chem. Soc.* 146, 20937–20944, 2024.

### PLENARY SPEAKER



#### Yuichi Negishi

Yuichi Negishi is a Professor at the Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University, in Sendai, Japan. He has studied metal nanoclusters since 1995, beginning with gas-phase clusters and the systematic isolation of glutathionate-protected gold nanoclusters, and developing precise techniques for controlling the size and structure of ligand-protected metal clusters. His current research applies these atomically precise clusters to the design of highly functional catalysts for energy and environmental applications. His honors include the PCCP Prize for Outstanding Achievement of Young Chemists in Physical Chemistry and the Best Young Presenter Award of the Society of Nano Science and Technology.

## Physicist in the Kitchen: Exploring the Gastronomic Universe

Andrey Varlamov<sup>1, 2</sup>

1) Institute of Superconductivity and Innovative Materials, Italian National Research Council, Rome, Italy

2) Lombard Institute “Academy of Sciences and Letters”, Milan, Italy

What governs the propagation of heat in food? Why does pizza baked in a traditional wood-fired oven taste different from one cooked in an electric oven? Why are boiled and grilled meats so distinct in flavor and texture? Can we scientifically determine the optimal cooking time for a soft-boiled duck egg or for spaghetti?

This lecture explores these and many other fascinating questions at the intersection of physics and gastronomy. We will discover why spaghetti usually breaks into three pieces rather than two, and how it can be made to snap in two; why a toast with crystal glasses filled with sparkling wine often lacks the expected resonant chime; why vodka typically contains about 40% alcohol; and why professional baristas adjust the grind size of coffee beans according to the weather.

By applying the principles of heat transfer, fluid dynamics, elasticity, acoustics, and thermodynamics to everyday culinary experiences, the lecture reveals the hidden physics behind the food we cook, eat, and enjoy. A journey through the gastronomic universe, viewed through the lens of a physicist.

---

### PLENARY SPEAKER



#### Andrey Varlamov

Andrey Varlamov is a principal investigator at the Institute of Superconductivity, Innovative Materials and Devices of the Italian National Research Council (CNR-SPIN). Born in Kyiv, he earned his PhD in condensed-matter physics in 1980 under Alex Abrikosov, later held professorships in Moscow and a fellowship at Argonne National Laboratory, and joined CNR in 1999. His research spans superconductivity, the theory of metals and phase transitions, thermoelectricity, and nanophysics; he co-authored the monograph "Theory of Fluctuations in Superconductors" with Anatoly Larkin and has published more than 200 papers. He received the USSR State Prize in Physics (1986) and the Bogolyubov Prize (2018), and his popular-science book "The Wonders of Physics" has appeared in sixteen editions and eight languages.

# Track 1

Nanomaterials Synthesis and Design

## Cohesive energy model for nanostructure formation on metal surfaces induced by slow highly charged ions

M. Majkić<sup>1</sup>\*

1) Faculty of Technical Sciences, University of Pristina in Kosovska Mitrovica, Serbia

\* milena.majkic AT pr.ac.rs

Slow highly charged ions (HCI) interacting with solid surfaces induce nanoscale modifications producing either hillocks or craters, depending on their potential and kinetic energy, as well as collision geometry [1]. Understanding these mechanisms is essential for advancing next-generation electronic and optoelectronic devices and controlled defect engineering.

In this contribution, I present a two-step cohesive energy model (CEM) predicting the formation of specific nanostructures by linking deposited energy to the resulting surface modification [2]. HCIs carry a substantial amount of potential energy, a portion of which is released as neutralisation energy upon neutralisation at the surface. Beneath the surface, the projectile slows down via interactions with atomic and electronic subsystems. The combined effect of kinetic energy loss and neutralisation energy, controlled by the critical ion velocity, determines the total energy deposited within a near-surface region.

The resulting nanostructure reflects the dominant contribution: hillocks and craters are associated with the neutralisation and kinetic energy dominance, respectively, while their coexistence occurs at the critical ion velocity. Varying the incidence angle reveals the existence of two energy regimes [2]: at low velocities, the process is driven by the critical ion velocity, whereas at higher velocities, the total deposited energy becomes the key parameter. In both regimes, decreasing the incidence angle enhances both energy contributions, resulting in higher total energy deposition, increasing the probability of crater formation. These predictions are consistent with experimental observations for highly charged Xe ions on titanium and gold surfaces, as well as with electron-yield data [3,4]. Using different ions highlights the role of core polarisation in surface modification. Stronger polarisation increases total deposited energy, favouring crater formation [5].

The results show that desired nanostructures can be intentionally created by tuning ion charge state, velocity, and incidence angle, providing a framework for controlled nanostructuring of metal surfaces.

---

**KEYWORDS:** Highly charged ions, Metal surface, Collision geometry, Surface nanostructure, Velocity effect

---

**ACKNOWLEDGEMENTS:** The author would like to thank the Ministry of Science, Technological Development and Innovation of the Republic of Serbia for funding the scientific research work, contract no. 451-03-65/2024-03/200155, realised by the Faculty of Technical Sciences in Kosovska Mitrovica, University of Pristina.

---

### REFERENCES

- [1] F. Aumayr *et al.*, *J. Phys.: Condens. Matter* 23, 39 (2011)
- [2] M. D. Majkić *et al.*, *Sci Rep* 15, 34457 (2025).
- [3] I. Stabrawa *et al.*, *Vacuum* 210, 111860 (2023)
- [4] W. Meissl *et al.*, *Nucl. Instrum. Methods Phys. Res. B* 256(1), 520-523 (2007)
- [5] M. D. Majkić *et al.*, *Phys. Status Solidi RRL*, 2500028 (2025)

## New insights into synthesis of inorganic nanotubes - solving the enigma of more than two decades of research

M. Krishnappa<sup>1,2</sup>, S. Ghosh<sup>1,3</sup>, Y. Feldman<sup>4</sup>, T. Livneh<sup>5</sup>, J. I. Martinez<sup>6</sup>, J. A. Alonso<sup>7</sup>, A. Zak<sup>1\*</sup>

1) Holon Institute of Technology, Israel

2) Nitte Meenakshi Institute of Technology, India

3) The Hebrew University of Jerusalem, Israel

4) Weizmann Institute of Science, Israel

5) Nuclear Research Center Negev, Israel

6) Institute of Materials Science of Madrid, Spain

7) University of Valladolid, Spain

\* alzak AT hit.ac.il

The breakthrough, enabled the reproducible one-pot synthesis of MoS<sub>2</sub> nanotubes (NTs) from molybdenum oxide via vapor-gas-solid (VGS) reaction, solved a two-decade enigma [1]. However, the reported process left some unresolved issues, such as how to increase the NT yield mixed with platelets beyond 30-40% and how to exclude defect-rich NTs. Here, I will report the successful completion of the first task by synthesizing phase-pure (100% yield) 1D MoS<sub>2</sub> nanotubes [2]. This progress was achieved through the development of a new synthesis for high-aspect-ratio MoO<sub>3</sub> nanowhiskers, the precursor for NTs production, and through careful study of the NTs' growth mechanism and the properties of the intermediate products of this multistep reaction. The synthesis of MoO<sub>3</sub> nanowhiskers was performed separately via a wet-chemistry process. Subsequently, the whiskers were served as a template for the preparation of nanotubes via a high-temperature, reduction/ sulfurization solid-gas reaction. The second task, synthesis of perfectly crystalline NTs was also achieved [2]. Perfectly crystalline NTs are well suited for electro-optical and electromechanical applications [3,4]. In parallel, it was discovered that defect-rich NTs, which have a high surface density of active sites and were initially considered unwanted, demonstrate superior performance as electrocatalysts for the hydrogen evolution reaction (HER) compared to perfectly crystalline NTs [5]. Therefore, our synthesis provides two types of NTs, perfectly crystalline and defect-rich, prepared under different conditions and in a controlled manner. To support advances in NT production and characterization, we sought for a deeper theoretical insight into the structural features of nanotubes, such as hollow core formation and interlayer distance discrepancies. Thus, the formation energy of the nanotubes was calculated from curvature strain, deformation and van der Waals energies, and the mechanism for changes in interlayer spacing was proposed. More specifically, optimizing the van der Waals interactions between incommensurately neighboring layers of the NTs via relaxation requires their expansion or contraction, thereby causing additional deformation within the layers. Thus, the interplay of all three energies influences the layer diameters and, thereby, the interlayer spacing. By integrating experiment and theory, we step forward toward broadening the application-oriented integration of MoS<sub>2</sub> NTs into devices

---

**KEYWORDS:** MoS<sub>2</sub>, MoO<sub>3</sub>, Perfect crystallinity, Defect-rich surface, Hydrogen evolution reaction

---

### REFERENCES

- [1] C. Pallelappa, S. Ghosh, A. Idelevich, L. Rovinsky, T. Livneh, A. Zak, Solving the "MoS<sub>2</sub> nanotubes" synthetic enigma and elucidating the route for their catalyst-free and scalable production, *ACS Nano*, 14, 3004 (2020)
- [2] M. Krishnappa, S. Ghosh, Y. Feldman, I. Lapsker, O. Brontvein, T. Livneh, J. Martinez, J.A. Alonso, A. Zak, Phase-pure MoS<sub>2</sub> nanotubes with controlled crystallinity, templated by pre-prepared high-aspect-ratio MoO<sub>3</sub> nanowhiskers, *ACS Nano*, 2026
- [3] Y.J. Zhang, T. Ideue, M. Onga, F. Qin, R. Suzuki, A. Zak, R. Tenne, J.H. Smet, Y. Iwasa, Letter: Enhanced intrinsic photovoltaic effect in tungsten disulphide nanotubes, *Nature*, 570, 349 (2019)
- [4] Y. Sun, S. Xu, Z. Xu, J. Tian, M. Bai, Z. Qi, Y. Niu, H.H. Aung, X. Xiong, J. Han, C. Lu, J. Yin, S. Wang, Q. Chen, R. Tenne, A. Zak, Y. Guo, Mesoscopic sliding ferroelectricity enabled photovoltaic random access memory for material-level artificial vision system, *Nature Communications*, 13, No.5391 2022
- [5] S.R. Kadam, K. Manjunath, S. Ghosh, M.B. Sreedhara, A. Neyman, A. Upcher, E. Nativ Roth, L. Houben, A. Zak, A.N. Enyashin, R. Bar-Ziv, M. Bar-Sadan, Nanotubes and other nanostructures of VS<sub>2</sub>, WS<sub>2</sub> and MoS<sub>2</sub>: Structural effects on the hydrogen evolution reaction, *Applied Materials Today*, 39, No.102288 (2024)

## Hexatic phase in covalent two- dimensional silver iodide

V. Skakalova<sup>1</sup>\*, T. T. A. Bui<sup>2</sup>, D. Lamprecht<sup>3</sup>, J. Madsen<sup>3</sup>, M. Kurpas<sup>4</sup>, P. Kotrusz<sup>5, 6</sup>, L. Filipovic<sup>7</sup>,  
J. C. Meyer<sup>8, 9, 2</sup>, K. Mustonen<sup>2</sup>

1) Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská cesta 9, 84104 Bratislava, Slovakia

2) Faculty of Physics, University of Vienna, Vienna, Austria

3) University of Vienna, Faculty of Physics, Boltzmannngasse 5, A-1090 Vienna, Austria

4) Institute of Physics, University of Silesia in Katowice, Poland

5) Danubia NanoTech S.r.o., Bratislava, Slovakia

6) Institute of Electrical Engineering and CEMEA SAS, Bratislava, Slovakia

7) Institute for Microelectronics, TU Wien, Vienna, Austria

8) Institute of Applied Physics, Eberhard Karls University of Tuebingen, Auf der Morgenstelle 10, D-72076, Tuebingen, Germany

9) Natural and Medical Sciences Institute at the University of Tuebingen, Markwiesenstr. 55, D-72770 Reutlingen, Germany

\* viera.skakalova AT univie.ac.at

In three-dimensional crystals, first-order phase transitions are characterized by discontinuous changes in thermodynamic quantities accompanied by the loss of crystal symmetries. In contrast, Kosterlitz- Thouless- Halperin- Nelson- Young (KTHNY) theory predicts that, in two dimensional crystals, the transition from a solid to liquid proceeds through an orientationally ordered “hexatic” phase in a continuous regime. However, some experimental observations suggest alternative, mixed melting scenarios, in which melting proceeds starting through the continuous hexatic phase, followed by discontinuous transitions.

Here we study a phase transition of two dimensional covalently bonded crystal of silver iodide embedded in multilayer graphene using scanning transmission electron microscopy (STEM) with atomic resolution and nanobeam electron diffraction. During heating up to 1200 °C, our in-situ time and temperature resolved measurements provide evidence for progressive formation of the hexatic phase approximately 25 °C below a sudden transition to the liquid phase, supporting the mixed melting scenario [1].

---

**KEYWORDS:** Two dimensional phase transitions, 2D silver iodide, Graphene, Hexatic phase, Transition scanning electron microscopy

---

**ACKNOWLEDGEMENTS:** V.S. has been supported by the V4- Japan Joint Research Program V4- Japan/JRP/2021/96/BGap Eng; grant no. VEGA 1/0104/25, provided by Ministry of Education, Research, Development, and Youth of the Slovak Republic, the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia, under project no. 09I05- 03- V02- 00071

---

### REFERENCES

- [1] T. A. Bui, D. Lamprecht, J. Madsen, M. Kurpas, P. Kotrusz, A. Markevich, C. Mangler, J. Kotakoski, L. Filipovic, C. Jannik. Meyer, Timothy J. Pennycook, Viera Skákalová, Kimmo Mustonen, Hexatic phase in covalent two- dimensional silver iodide, SCIENCE, 7915 (2025), science.org/doi/10.1126/science.adv7915

## First-principles investigation of defects in hexagonal-diamond silicon

M. Amato<sup>1\*</sup>, P. Muchiri<sup>2</sup>, M. Túnica<sup>3</sup>, A. Marzegalli<sup>4</sup>, E. Scalise<sup>4</sup>, F. Chiodi<sup>5</sup>, A. Zobelli<sup>6</sup>

1) Laboratoire de Physique des Solides Université Paris-Saclay, France

2) Laboratoire de Physique des Solides, Université Paris-Saclay, France

3) Technische Universität Darmstadt, Germany

4) Department of Materials Science, Università di Milano Bicocca, Italy

5) Centre de Nanosciences et de Nanotechnologies, Université Paris-Saclay, France

6) Laboratoire de Physique des Solides Université Paris-Saclay, France

\* michele.amato AT universite-paris-saclay.fr

Recent progress in the synthesis and characterization of hexagonal-diamond silicon (2H-Si) in the form of nanowires [1] has highlighted its distinct structural, electronic, and optical properties compared to the conventional cubic-diamond (3C-Si) phase. While the physical properties of 2H-Si have been widely investigated, the role of impurities in this phase remains largely unexplored, particularly in the high-doping regime. In this work, we present results from density functional theory (DFT) simulations examining the effects of substitutional doping in 2H-Si and comparing them with those in the 3C phase.

We analyze both p-type and n-type dopants, exploring their behavior in neutral and charged states [2,3]. Our simulations reveal that impurities in 2H-Si adopt different local symmetries compared to those in 3C-Si, reflecting the influence of the host crystal structure. For acceptors, we find that 2H-Si exhibits lower formation energies and shallower charge transition levels than the cubic phase, making p-type doping more favorable in the hexagonal structure. Conversely, n-type dopants show lower formation energies and transition levels in 3C-Si, suggesting more efficient electron activation in the cubic phase. These trends persist even in the ultra-high doping regime [4].

Building on these insights, we employ a band-offset diagram for the 2H and 3C polytypes to propose a model in which hole doping can energetically stabilize the 2H phase. This provides a potential strategy for phase engineering via carrier injection [3]. These findings also lay the groundwork for understanding dopant interactions with stacking faults in 2H-Si [5].

Overall, this work provides new insight into doping behavior in non-cubic group-IV nanostructures, which is essential for enabling 2H-Si applications in future optoelectronic and quantum devices.

---

**KEYWORDS:** Defects, Hexagonal-diamond silicon, Semiconductor, DFT, Ab initio

---

**ACKNOWLEDGEMENTS:** We acknowledge the ANR project AMPHORE (ANR-21-CE09-0007) and the ANR project TULIP (ANR-24-CE09-5076). Part of the high-performance computing resources for this work were granted by the Institut du Développement et des Ressources en Informatique Scientifique (IDRIS) under the allocations AD010914974 and AD010915077 via GENCI (Grand Equipement National de Calcul Intensif).

---

### REFERENCES

- [1] E.M.T. Fadaly, A. Dijkstra, J.R. Suckert, *et al.* Direct-bandgap emission from hexagonal Ge and SiGe alloys. *Nature* 580, 205-209 (2020)
- [2] M. Amato, S. Ossicini, E. Canadell, R. Rurali, Preferential positioning, stability, and segregation of dopants in hexagonal Si nanowires, *Nano Lett.*, 19 (2), 866-876 (2019)
- [3] M. Túnica, A. Zobelli, M. Amato, Acceptor and donor impurity levels in hexagonal-diamond silicon, *Phys. Rev. Mater.*, 8, 114601 (2024)
- [4] M. Túnica, F. Chiodi, M. Amato, Structural and thermodynamic stability in hexagonal-diamond SiGeB alloys, *Semicond. Sci. Technol.* 41 (1), 015005 (2026)
- [5] P. W. Muchiri, A. Zobelli, A. Marzegalli, E. Scalise, M. Amato, Interaction of Dopants with the I-Type Basal Stacking Fault in Hexagonal-Diamond Si, *J. Phys. Chem. C* 129 (24), 11093-11 (2025)

## Impact of post-synthesis atmosphere on the PEC behavior of semitransparent Cu-functionalized TiO<sub>2</sub> nanotubes

K. Grochowska<sup>1\*</sup>, S. I. Khan<sup>1</sup>, W. Lipińska<sup>1</sup>, J. Karczewski<sup>2</sup>, K. Załęski<sup>3</sup>, E. Coy<sup>3</sup>, J. Gumieniak<sup>4</sup>,  
A. Kramek<sup>4</sup>, K. Siuzdak<sup>1</sup>

1) Centre for Plasma and Laser Engineering, the Szewalski Institute of Fluid-Flow Machinery, Polish Academy of Sciences, Fiszerza 14 St., 80-231 Gdańsk, Poland, Poland

2) Gdańsk University of Technology, Poland

3) NanoBioMedical Centre, Adam Mickiewicz University, ul. Wszechnicy Piastowskiej 3, 61-614 Poznan, Poland

4) Rzeszow University of Technology, Poland

\* kgrochowska AT imp.gda.pl

The growing global demand for energy, together with the escalating impacts of climate change, highlights the urgent need for sustainable and efficient energy conversion solutions. Solar energy stands out as a clean, abundant, and renewable resource with strong potential to reduce environmental burden while supporting long-term energy sustainability. Among various solar energy conversion approaches, photoelectrochemical (PEC) systems have attracted significant attention due to their ability to directly convert solar energy into electricity or chemical fuels. Titanium dioxide is one of the most widely studied materials in PEC applications, owing to its excellent chemical stability, mechanical robustness, and cost-effectiveness. Nevertheless, its relatively wide bandgap (approximately 3.2 eV for anatase) limits light absorption mainly to the ultraviolet region, which significantly constrains its overall efficiency. Therefore, strategies aimed at improving the photoactivity of TiO<sub>2</sub> are of considerable interest.

In this work, semitransparent Cu-modified titania nanotube electrodes were prepared by anodizing TiCu co-deposited films and by controlled annealing under air and hydrogen atmospheres. Structural and compositional analyses confirmed the formation of well-aligned nanotube arrays, with distinct distribution of copper nanoparticles in hydrogen-annealed samples and presence of copper oxide species in air-annealed samples. The UV-vis spectra revealed that the absorption band is shifted towards the visible range beyond 400 nm. Additionally, the hydrogen-annealed material demonstrates the highest photocurrent densities, reaching 7  $\mu\text{A cm}^{-2}$  under UV-vis illumination and 3.5  $\mu\text{A cm}^{-2}$  under visible light (at +0.1 V vs. Ag/AgCl/0.1 M KCl), which is approximately 5 times higher in UV-vis and 7 times higher in the visible region compared to the H<sub>2</sub>-annealed bare titania. Moreover, the electrode with the highest Cu loading exhibited the highest oxygen evolution reaction (OER) current density of 2.2 mA cm<sup>-2</sup> at +1.3 V vs. Ag/AgCl/0.1 M KCl, accompanied by intensive gas evolution. Overall, the semitransparent Cu-modified titania nanotube electrodes demonstrate photoactivity and OER performance, suggesting their suitability for applications where light transmission and electrochemical activity are both required.

---

**KEYWORDS:** Semitransparent materials, Oxide nanotubes, Oxygen evolution reaction

---

**ACKNOWLEDGEMENTS:** The authors acknowledge the financial support of the National Science Centre (Poland) via grant no: 2021/41/B/ST8/01849.

## Tuning electrochemical synthesis parameters to create porous oxide layers with complex channel structures

A. A. Świerkula<sup>1, 2 \*</sup>, L. Zaraska<sup>3</sup>

1) Department of Physical Chemistry and Electrochemistry, Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Krakow, Poland; Doctoral School of Exact and Natural Sciences, Jagiellonian University, Lojasiewicza 11, 30-348 Krakow, Poland., Poland

2) Doctoral School of Exact and Natural Sciences, Jagiellonian University, prof. S. Łojasiewicza 11, 30-348 Kraków, Poland., Poland

3) Department of Physical Chemistry & Electrochemistry, Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Krakow, Poland, Poland

\* aleksandra.swierkula AT doctoral.uj.edu.pl

Anodic oxidation (anodization) is a widely used method for producing nanostructured metal oxides. Anodic Aluminum Oxide (AAO), formed in this process, is broadly applied due to the ability to precisely control its morphology through electrochemical parameters such as voltage and electrolyte type. Process modifications, including lowering the applied voltage or using phosphoric acid-based electrolytes at relatively low voltages, enable the formation of oxide layers with complex channel geometries, such as Y-shaped[1,2] or serrated pores. The choice of electrolyte also significantly influences the optical properties of both the AAO layer and the underlying aluminum surface. Anodization in organic acids (e.g., malic, citric, or etidronic acid) results in oxide layers with rainbow-like coloration, while phosphoric acid produces milky films. Additionally, pore ordering can be tuned by employing mixtures of different acids[3].

This work discusses the selection of anodization conditions for obtaining AAO layers with complex channel geometries, particularly Y-shaped and serrated structures. AAO was fabricated on aluminum foil using various acid solutions and water-alcohol mixtures as electrolytes. Results show that combining different acids, along with adjustments in voltage and hydrodynamic conditions, enables the formation of channels with complex geometries. The development of nanostructured surface topography on aluminum during anodization is also addressed.

---

**KEYWORDS:** Anodization, Anodic alumina, Nanoporous layers, Channels with complex geometries

---

**ACKNOWLEDGEMENTS:** The research was carried out under the Sonata Bis project financed by the National Science Centre, Poland (no 2018/30/E/ST5/00531). The SEM imaging was performed in the Laboratory of Field Emission Scanning Electron Microscopy and Microanalysis at the Institute of Geological Sciences, Jagiellonian University, Poland.

---

### REFERENCES

- [1] L. Zaraska, E. Kurowska, G. D. Sulka, and M. Jaskuła, "Porous alumina membranes with branched nanopores as templates for fabrication of Y-shaped nanowire arrays", *J. Solid State Electrochem.*, 16, 3611-3619 (2012).
- [2] A. Świerkula, and L. Zaraska, "The use of sulfuric and oxalic acid mixtures to obtain AAO layers with different channel geometries", *J. Phys.: Mater.*, 9, 015012, (2026).
- [3] A. Świerkula, and L. Zaraska, "Tuning the geometry of porous alumina layers via anodization in mixtures of different acids" *Journal of Solid State Electrochemistry*, *J. Solid State Electrochem.*, 29, 1449-1458, (2025).

## High-performance arsenic-free selector-only memory enabled by trap-state engineering in Sb-doped Ge<sub>2</sub>Se<sub>3</sub>

S. Kim<sup>1</sup>\*, H. Sung<sup>1</sup>, H. Lee<sup>1</sup>

*1) Korea University, Republic of Korea*

\* tldn0303 AT korea.ac.kr

Next-generation storage-class memory (SCM) requires high density and low power consumption. Selector-only memory (SOM) is a leading candidate because it integrates both selector and memory functions into a single chalcogenide layer, enabling highly scalable and multi-stackable 3D crossbar arrays. However, most SOM materials rely on toxic arsenic (As), which limits their use in large-scale semiconductor manufacturing. To overcome this, we developed an As-free Sb-doped Ge<sub>2</sub>Se<sub>3</sub> SOM device that is both environmentally friendly and CMOS-compatible.

The devices were fabricated using an industry-compatible co-sputtering process. Our core strategy focuses on trap-state engineering rather than simple composition tuning. By systematically varying the Sb concentration (0 to 21 at%), we identified 16 at.% Sb as the optimal doping level. This strategic doping modifies the local Ge-Se bonding network to create optimized shallow trap states. This engineered environment stabilizes hole transport and field-induced threshold switching, resulting in a significantly more reliable switching operation. Structural analyses using TEM, XRD, and XPS confirm that Sb doping enhances the thermal and physical stability of the amorphous phase. Specifically, Sb suppresses structural relaxation at temperatures up to 350°C, which is directly linked to improved endurance and reduced threshold voltage (V<sub>th</sub>) drift. We also observed that excessive doping (>21 at.%) leads to the formation of Sb clusters. These nanoclusters cause carrier scattering and degrade transport symmetry, proving that precise nanoscale control of Sb concentration is critical for performance.

The optimized 16 at.% Sb-doped SOM device achieved outstanding electrical characteristics: a wide memory window (MW) of 2.3 V, an ultra-low leakage current of ~20 nA, and superior V<sub>th</sub> stability. These results demonstrate a significant improvement over undoped Ge<sub>2</sub>Se<sub>3</sub> devices in terms of power efficiency and operational reliability. This study confirms that trap-state engineering in As-free chalcogenides is a highly effective and scalable path for the next generation of high-density 3D data storage solutions.

---

**KEYWORDS:** Selector-Only memory (SOM), As-free, Trap-state engineering, Sb-doped Ge<sub>2</sub>Se<sub>3</sub>, 3D crossbar array

---

**ACKNOWLEDGEMENTS:** This research was supported by the Nano & Material Technology Development Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science and ICT (RS-2025-02217649).

---

### REFERENCES

- [1] S. Hong, H. Choi, J. Park, Y. Bae, K. Kim, W. Lee, S. Lee, H. Lee, S. Cho, J. Ahn, S. Kim, T. Kim, M. Na, and S. Cha, IEEE Symp. VLSI Technol. (2022) 1.

## First principle study of spontaneous polarization due to Co and V substitution in wurtzite AlN

A. Moitra<sup>1</sup>\*, A. Soni<sup>1</sup>, A. Gunjesh<sup>1</sup>, A. Chauhan<sup>1</sup>

1) Delhi Technological University, India

\* abhroneel.moitra AT gmail.com

Spontaneous polarization is an emerging area in modern electronics owing to its application in various fields especially in high speed transistor operations. Ferroelectric materials exhibit spontaneous polarization due to spatial displacement between centers of positive and negative charges. Often spontaneous polarization is linked to piezoelectricity due to its sensitive dependency on mechanical stress and temperature[1] making these materials useful for acoustics and various actuators as well. While most ferroelectric materials are perovskite oxides, recently wurtzite related materials like YbAlN[2] and ScAlN[3] have been also emerging as viable alternatives. This paper investigates the spontaneous polarization of wurtzite Aluminium Nitride (AlN) structures substituted with transition metals Cobalt and Vanadium using first-principles calculations. Five structures were chosen for each metal at substitution concentrations of 25% and 50%. Peak spontaneous polarization of 0.216 C/m<sup>2</sup> and 0.271 C/m<sup>2</sup> were achieved at 25% substitution of Vanadium and 50% substitution of Cobalt in wurtzite AlN respectively. This depicts a substantial enhancement compared to the calculated value of -0.1229 C/m<sup>2</sup> for pristine AlN[4]. This has been mainly achieved through the distortions of the lattice structure and the changes in the bond length between metal and nitrogen atoms along the c-axis[5]. The negative value of the total energy obtained for all these structures is an indication of their stability. This makes V and Co-substituted Aluminum Nitride a potential substitute for polarization purposes, especially in the production of GaN HEMT, FeFET, and RF filters.

**KEYWORDS:** CoAlN, VAlN, First-principles calculation, Spontaneous polarization, High-electron-mobility transistors

### REFERENCES

- [1] M. Akiyama, K. Kano, and A. Teshigahara, “Influence of growth temperature and scandium concentration on piezoelectric response of scandium aluminum nitride alloy thin films,” *Applied Physics Letters*, vol. 95, no. 16, p. 162107, October 2009.
- [2] K. Hirata, S. Kawano, H. Yamada, M. Uehara, S. A. Anggraini, and M. Akiyama, “Spontaneous polarization and polarization-induced electron sheet charge of YbAlN on GaN: A first-principles study,” *Japanese Journal of Applied Physics*, vol. 60, no. SB, p. SBBA05, March 2021.
- [3] M. A. Caro, S. Zhang, M. Ylilammi, T. Riekkinen, M. A. Moram, O. Lopez-Acevedo, J. Molarius, and T. Laurila, “Piezoelectric coefficients and spontaneous polarization of scandium aluminum nitride (ScAlN) alloys,” *Journal of Physics: Condensed Matter*, vol. 27, no. 24, p.245901, June 2015.
- [4] F. Bernardini, V. Fiorentini, and D. Vanderbilt, “Spontaneous polarization and piezoelectric constants of III-V nitrides: A first-principles study,” *Physical review B*, vol. 56, no. 16, pp. R10024-R10027, October 1997.
- [5] R. D. King-Smith and D. Vanderbilt, “Theory of polarization of crystalline solids,” *Physical Review B*, vol. 47, no. 3, pp. 1651-1654, January 1993.

## From nanoscale polymer chain dynamics to dielectric response: DMA-tuned pH-responsive hydrogels

E. Bilgen<sup>1</sup>, V. Can<sup>1</sup>, S. Dumanli<sup>2</sup>, Z. C. C. Ozdil<sup>1</sup> \*

1) Yeditepe Universtiy, Turkey

2) Bogazici University, Turkey

\* cansu.canbek AT yeditepe.edu.tr

pH-responsive hydrogels have attracted significant interest for implantable sensory systems due to their ability to undergo substantial water uptake and to exhibit tunable swelling responses to environmental stimuli, leading to detectable changes in their physicochemical properties [1]. Acrylamide and acrylic acid (AAM-AAc) based hydrogels exhibit swelling behavior moderated by the ionization of carboxylic groups, enabling tuneable response to environmental pH stimuli [1]. Additionally, swelling, mechanical properties, and transport characteristics of hydrogels can be effectively tuned through monomer composition and network structure [2]. However, for dielectric based sensing applications, the high water content of such systems can limit signal contrast with the surrounding biological environment, as the dielectric response is largely governed by water dipole polarization, thereby suppressing nanoscale contributions arising from polymer chain conformation and network structure, which require molecular-level analysis to be resolved.

In this study, we investigate the effects of incorporating N,N-dimethylacrylamide (DMA) as a non-ionic comonomer on the swelling behavior, dielectric, and mechanical properties of P(AAm-co-AAc-co-PEGDA) matrix. A combined experimental and computational approach is employed, in which molecular-level conformational changes in the polymer network are analyzed using LAMMPS simulations to estimate the radius of gyration ( $R_g$ ), enabling correlation between nanoscale chain behavior and macroscopic swelling response. Hydrogels were synthesized via free-radical polymerization and characterized by pH-dependent swelling, mechanical testing, and permittivity measurements. Three formulations were prepared: (1) AAm/AAc = 90/10, (2) AAm/AAc/DMA = 89/10/1, and (3) 80/10/10 mol%.

For mechanical tests and permittivity readings, a new synthesis protocol is developed to produce homogeneous thin layers 1.5mm thick, allowing direct rheological characterization. Rheological analysis revealed that the mechanical properties of AAm-AAc based hydrogels decrease with increasing DMA concentration. Formulations (1) and (3) exhibited relatively consistent storage modulus values of approximately 17,000 Pa and 11,000 Pa, respectively, whereas formulation (2) showed more variable values in the range of 13,000-15,000 Pa. This variability is attributed to the insufficient DMA content, which likely led to inhomogeneous dispersion within the polymer network.

Swelling analysis showed that the overall swelling capacity of AAm-AAc-based hydrogels decreases with increasing DMA concentration, without affecting the pH-dependent swelling behavior of the system. These experimental findings are qualitatively supported by LAMMPS-based nanoscale molecular simulations, which indicate reduced polymer chain expansion with increasing DMA content, as reflected by decreased  $R_g$  values.

---

**KEYWORDS:** PH-responsive hydrogels, Nanoscale chain dynamics, Dielectric properties

---

### REFERENCES

- [1] G. Patroklou, E. Triantafyllopoulou, P.E. Goula, V. Karali, M. Chountoulesi, G. Valsami, S. Pispas, N. Pippa, pH-Responsive Hydrogels: Recent Advances in Pharmaceutical Applications. *Polymers* 2025, 17 (11), 1451. <https://doi.org/10.3390/polym17111451>.
- [2] R. Wang, C. Cheng, H. Wang, D. Wang, Swollen Hydrogel Nanotechnology: Advanced Applications of the Rudimentary Swelling Properties of Hydrogels. *ChemPhysMater* 2024, 3 (4), 357-375. <https://doi.org/10.1016/j.chphma.2024.07.006>.

## Spark ablation of Cu<sub>(x)</sub>O nanoparticles: Size and phase control

D. Mereib<sup>1</sup>\*, J. ElRifai<sup>2</sup>, E. Bsaibess<sup>2</sup>, M. Zaghrioui<sup>3</sup>

1) Sorbonne Abu Dhabi University, United Arab Emirates

2) SUAD Research Institute, Sorbonne University Abu Dhabi, Abu Dhabi, United Arab Emirates, United Arab Emirates

3) GREMAN, UMR 7347 - CNRS, IUT de Blois, University of Tours, 15 Rue de la Chocolaterie, CEDEX, 41029, Tours, Blois, France, France

\* diaa.mereib AT sorbonne.ae

Copper oxide nanoparticles Cu<sub>(x)</sub>O have attracted significant interest due to their catalytic, antimicrobial, and electronic functionalities. At the nanoscale, these materials exhibit increased surface activity along with tunable optical and electrical characteristics, which makes them highly suitable for use in environmental, sensing, energy-related applications, and biomedical applications [1]. A key challenge remains the precise regulation of particle size, phase composition, and aggregation state in order to optimize performance while ensuring sustainable synthesis routes.

In this work, a completely dry spark ablation technique is utilized to synthesize Cu<sub>(x)</sub>O nanoparticles directly from copper electrodes, without chemical precursors or solvents [2]. Each electrical discharge vaporizes a small volume of copper, which is then rapidly cooled in a nitrogen carrier gas, forming a continuous aerosol of nanoparticles typically in the range of 2-20 nm. By adjusting parameters such as carrier gas flow rate and ablation time, the study investigates their impact on particle nucleation, growth mechanisms, spatial distribution of clusters on the substrate, and agglomeration dynamics.

The nanoparticles are systematically characterized using complementary analytical techniques to elucidate their structure and composition. Scanning Electron Microscopy coupled with Energy Dispersive Spectroscopy (SEM-EDS) is employed to examine particle morphology and elemental composition. Raman spectroscopy and transmission electron microscopy (TEM), supported by selected area electron diffraction (SAED), are used to identify copper oxide phases through vibrational signatures and crystallographic analysis, respectively, while enabling the distinction between Cu<sub>x</sub>O phases.

The findings highlight that spark ablation represents a fast, controllable, and eco-friendly approach for producing Cu<sub>(x)</sub>O nanoparticles with adjustable size, aggregation characteristics, and phase composition. The precursor-free nature of the method, together with precise parameter control, establishes this method as a sustainable and efficient route for fabricating copper oxide nanomaterials applicable across diverse technological and biomedical fields.

---

**KEYWORDS:** Spark ablation, Copper oxide nanoparticles, Size control, Phase control, Aerosol synthesis

---

**ACKNOWLEDGEMENTS:** Spark ablation, Copper oxide nanoparticles, Dry synthesis, Size and phase control

---

### REFERENCES

- [1] B. D. Harishchandra *et al.*, “Copper Nanoparticles: A Review on Synthesis, Characterization and Applications,” *Asian Pac. J. Cancer Biol.*, vol. 5, no. 4, pp. 201-210, Dec. 2020, doi: 10.31557/apjcb.2020.5.4.201-210.
- [2] N. S. Tabrizi, M. Ullmann, V. A. Vons, U. Lafont, and A. Schmidt-Ott, “Generation of nanoparticles by spark discharge,” *J. Nanoparticle Res.*, vol. 11, no. 2, pp. 315-332, Feb. 2009, doi: 10.1007/s11051-008-9407-y.

## Microwave-engineered carbon composites for adaptive thermal management

J. Zhu<sup>1</sup>\*, Y. Hu<sup>1</sup>, J. Hu<sup>1</sup>

1) Nanjing University of Science and Technology, China

\* 19zhujun AT njust.edu.cn

Adaptive thermal management materials are of great interest for infrared camouflage, wearable thermal protection, and electronic heat regulation. Herein, we present an integrated study on microwave-engineered carbon composites, focusing on silver-carbon interfacial regulation, phase-change microcapsule design, and hydrogel/aerogel thermal management platforms. First, Ag nanoparticles were constructed on graphene oxide (GO), carbon nanotubes (CNTs), and GO/CNT hybrid substrates. Under microwave irradiation, carbon defects, oxygen-containing groups,  $\pi$ -conjugated domains, and localized microwave absorption jointly promoted Ag nucleation, anchoring, and interfacial coupling. GO provided planar defect sites for Ag growth, CNTs offered curved active sites and local microwave-absorbing regions, while GO/CNT hybrid networks established three-dimensional frameworks for Ag stabilization and anisotropic heat transport.

The substrate-dependent Ag-carbon interfaces enabled efficient thermal regulation after being assembled into porous or flexible matrices. For Ag/GO aerogels, the CCB-SCP/Chitosan composite showed a low density of 0.064 g·cm<sup>-3</sup>, an ultra-low thermal conductivity of 0.018 W·m<sup>-1</sup>·K<sup>-1</sup>, and a thermal shielding temperature difference of approximately 50 °C; under a 190 °C heating platform, the apparent surface temperature decreased to 144.0 °C [1]. For Ag/CNT aerogel systems, the optimized Ag<sub>25</sub>wt%-CNT/PVA aerogel exhibited a thermal conductivity of 0.115 W·m<sup>-1</sup>·K<sup>-1</sup>. After further integration with a PEG phase-change layer and an ITO low-emissivity film, the bioinspired multilayer composite reached a stable surface temperature of only 48.2 °C on a 200 °C platform, together with a PEG melting enthalpy of 171.4 J·g<sup>-1</sup> and low ITO emissivities of 0.144 and 0.112 in the 3-5 and 8-14  $\mu$ m bands, respectively [2]. Preliminary Ag-carbon hydrogel studies also indicated that Ag-CNT/PVA/Glc hydrogels could combine flexibility and infrared regulation, showing a fracture elongation up to 166.5% and thermal camouflage behavior under a 65 °C background.

In addition, PEG@SiO<sub>2</sub> microcapsules were investigated as phase-change units for latent-heat buffering. Microwave-assisted PEG@SiO<sub>2</sub> encapsulation was explored as a rapid preparation route, but the best preliminary sample only showed an encapsulation ratio/efficiency of approximately 71.4%/69.9%, which decreased after thermal cycling, indicating insufficient shell stability. In contrast, optimized emulsion/sol-gel-derived PEG@SiO<sub>2</sub> microcapsules achieved an encapsulation efficiency of 88.86% and enabled TEMPS hydrogels to maintain surface temperatures of 28.5, 31.7, and 37.4 °C under 38.5, 55, and 75 °C heating, respectively [4]. Overall, this work highlights the structure-property relationships among microwave-induced Ag-carbon interfaces, phase-change buffering, and flexible porous matrices, providing a feasible strategy for adaptive thermal management.

---

**KEYWORDS:** Microwave synthesis, Carbon composites, Silver-carbon interfaces, Phase-change microcapsules, Thermal management

---

### REFERENCES

- [1] J. Hu, Y. Hu, J. Yang, Y. Ye and R. Shen, “Nano-assembled modified graphene composites based on rapid microwave fabrication for thermal management”, *Chem. Eng. J.*, 476, (2023) p. 146670.
- [2] J. Zhu, Y. Hu, J. Hu, B. Zhou, Y. Ye and R. Shen, “Bioinspired Multilayer Composites Based on Nano-Self-Assembled Thermomechanical Expressway for Efficient Thermal Management”, *Small*, 21, (2025) p. 2412452.
- [3] J. Hu, J. Zhu, Y. Hu, J. Yang, Y. Ye and R. Shen, “Interface-Driven Construction of Three-Dimensional Silver-Carbon Aerogels via Microwave Radiation for Thermal Regulation”, *J. Mater. Chem. A*, (2026), DOI: 10.1039/D5TA09196A.
- [4] J. Zhu, Y. Hu, Z. Wu, J. Hu, X. Pei, Y. Dong, P. Wang, H. Li, B. Zhou, Y. Ye and R. Shen, “Bioinspired thermo-electro-mechanical phase-change system hydrogels for robust adaptive coupled functionality”, *Nano Energy*, 153, (2026) p. 111921.

## Plant-mediated synthesis of iron nanoparticles: Properties and application in latent fingerprint detection

F. H. Thaha<sup>1</sup>\*, M. F. Folkestad<sup>1</sup>, G. S. Khokhar<sup>1</sup>, N. K. S. Raghav<sup>2</sup>, N. Singh<sup>1</sup>

1) Amity University Dubai, United Arab Emirates

2) Bihar State Forensic Science Laboratory, Patna, India, India

\* fathima\_127 AT hotmail.com

Latent print detection remains a crucial biometric component in both forensic science and criminal investigation procedures. Traditional fingerprint powders, especially black powder, are widely used despite their low sensitivity and environmental and toxic hazards, which demonstrate the necessity for sustainable alternatives [1-2]. The high reactivity and expansive surface area of nanoparticles demonstrate substantial potential for latent fingerprint detection. New investigations have demonstrated that the ability of nanoparticles to visualize latent fingerprints depends on their size, shape, and stability [3]. This research focuses on biosynthesizing and examine iron nanoparticles (FeNPs) from aqueous extracts of fermented black tea (*Camellia sinensis*) and green tea (*Camellia sinensis*) for use in developing latent fingerprints. Tea phytochemicals containing polyphenols and flavonoids allow for the green production of uniformly distributed iron nanoparticles under alkaline pH conditions using ammonia solution. The particle size of biosynthesized iron nanoparticles was confirmed through initial characterization with Dynamic Light Scattering (DLS) and UV-Vis spectrophotometry. The average particle size determined by DLS is around 20-25 nm. The application of activated nanoparticles showed strong attachment to fingerprint residues on non-porous surfaces, resulting in clearer ridge patterns visualization and higher contrast images, which notably outperformed conventional black fingerprint powders. The results from this research demonstrate how tea-based green synthesis can create iron nanoparticles with promising applications for latent fingerprint development. The green method reduces chemical waste and health hazards found in standard approaches while providing an affordable, sustainable solution for nanomaterial production. Further studies will assess biosynthesized nanoparticles function across different surfaces in terms of sensitivity and durability while measuring performance levels.

---

**KEYWORDS:** Green synthesis, Black tea, Green tea, Iron nanoparticles, Forensics applications

---

**ACKNOWLEDGEMENTS:** Our sincere thanks to Amity University Dubai for providing the opportunity and resources to acquire firsthand learning and work experience.

---

### REFERENCES

- [1] S.A. Sari, U. Qalbiah, I.C. Putri, “Comparison between latent fingerprint identification using black powder and cyanoacrylate glue”, *Asian. J. Chem.* 30:2615-2620 (2018).
- [2] C. Lennard, “Forensic Sciences - Fingerprint Techniques”, *Encyclopedia Anal. Sci.*, 38 - 47 (2019).
- [3] N.K.B. Lotey, R. Lemos, F. D’Silva, A. Deshmukh, N. Singh, S. Wankhede, R. Davuluri, N. Vishe, and S. Kulkarni, “Highly Fluorescent Bio-Synthesized Carbon Quantum Dots for Latent Fingerprint Detection”, *J. Fluoresc.* (2025). <https://doi.org/10.1007/s10895-024-04107-8>

## Tunable visible emission from CdZnSe-CdZnS alloy nanorods via Cu-mediated cation exchange

V. Chaudhary<sup>1\*</sup>, S. Sivakumar<sup>1</sup>

*1) Indian Institute of Technology Kanpur, India*

\* vivekch AT iitk.ac.in

The anisotropic geometry of CdS-CdSe nanorods facilitates linearly polarized photoluminescence (PL) emission, making them attractive for optoelectronic applications. Considerable efforts have been devoted to incorporating various metal components into these nanostructures to enhance their functionality. Here, we demonstrate a Cu-catalyzed cation exchange strategy that enables the transformation of CdS-CdSe nanorods into CdZnS-CdZnSe alloy nanorods while preserving their original size, shape, and crystal structure. The ability to tailor composition and engineer core/shell heterostructures has expanded the tunability of optical properties in colloidal semiconductor nanocrystals. However, controlled alloying and heterostructure formation in anisotropic nanorods remain particularly challenging. The development of nanorods with broad spectral tunability is crucial for applications such as biological imaging, photovoltaics, light-emitting diodes, and next-generation display technologies. In this work, we report the synthesis of CdZnS-CdZnSe alloy nanorods via a Cu-assisted solid-solution alloying process, starting from CdS-CdSe nanorods. The resulting alloyed nanorods exhibit tunable photoluminescence spanning 480-650 nm while maintaining high emission intensity and structural uniformity. We attribute this alloying process to the high mobility of Cu cations within the Cd-chalcogenide lattice at elevated temperatures, which facilitates the controlled incorporation of Zn while preserving the anisotropic morphology. This study not only presents a robust route for the synthesis of high-quality alloy nanorods with precisely engineered optical properties but also paves the way for advancing alloy-based heteronanostructures for diverse optoelectronic and bioimaging applications.

---

**KEYWORDS:** Nanorods, CdS-CdSe, Cation exchange, Alloying, Cadmium chalcogenides

---

**ACKNOWLEDGEMENTS:** The authors acknowledge Department of Chemical Engineering, IIT Kanpur for providing financial assistance and fellowship received from the M.H.R.D, Government of India.

---

### REFERENCES

- [1] O. Chen, J. Zhao, V.P. Chauhan, J. Cui, C. Wong, D.K. Harris, H. Wei, H.S. Han, D. Fukumura, R.K. Jain, M.G. Bawendi, Compact High-Quality CdSe-CdS Core-Shell Nanocrystals with Narrow Emission Linewidths and Suppressed Blinking. *Nature Materials* 2013 12:5 2013, 12 (5), 445-451.
- [2] Y. Jiang, S.Y. Cho, M. Shim, Light-Emitting Diodes of Colloidal Quantum Dots and Nanorod Heterostructures for Future Emissive Displays. *Journal of Materials Chemistry C*. 2018.
- [3] G.A. Drake, J.C. Flanagan, M. Shim, Highly Luminescent Double-Heterojunction Nanorods. *Journal of Chemical Physics* 2019, 151 (13).
- [4] B.C. Steimle, J.L. Fenton, R.E. Schaak, Rational Construction of a Scalable Heterostructured Nanorod Megalibrary. *Science* (1979) 2020, 367 (6476).
- [5] B. Ji, Y.E. Panfil, N. Waiskopf, S. Remennik, I. Popov, U. Banin, Strain-Controlled Shell Morphology on Quantum Rods. *Nat Commun* 2019, 10 (1).

## Green-synthesized copper nanoparticles for functional latent fingerprint visualization: A nanomaterials approach

S. Sijo<sup>1\*</sup>, S. Sameer<sup>1</sup>, G. S. Khokhar<sup>1</sup>, N. K. S. Raghav<sup>2</sup>, N. Singh<sup>1</sup>

1) Amity University Dubai, United Arab Emirates

2) Bihar State Forensic Science Laboratory, Patna, India, India

\* alphymary01 AT gmail.com

Fingerprints represent one of the most reliable and persuasive sources of forensic investigations. Development of such latent prints has long depended upon the use of powders and chemicals effective as these, but which all too frequently necessitate the consideration of the issue of toxicity, cost, and environmental consequence [1]. Forensic nanotechnology has become a promising solution to address these issues. The unique physicochemical characteristics and high surface area-to-volume ratio of nanoparticles enable improved selectivity and sensitivity for latent fingerprint detection [2]. Plant-based green synthesis methods produce nanoparticles that have gained interest for their lower toxicity levels, cost efficiency, biodegradability and ability to meet sustainable forensic science objectives [3].

The aim of our present research is to develop a sustainable solution to biosynthesize copper nanoparticles (CuNPs) with the use of the natural, ubiquitous waste material, mandarin peel. Mandarin peels abound with phytochemicals such as flavonoids, polyphenols, essential oils, as well as organic acids. Such phytochemicals fulfil two functions in our biosynthesis, they act as natural reducing agents to synthesize the copper ions into the nanoparticle form, as well as stabilizing agents to inhibit agglomerations in the particles. We used copper (II) chloride dehydrate as a metal precursor and mixed it with mandarin peel powder in controlled environment conditions to successfully produce viable copper-based nanoparticles (CuNPs). The process is not only chemically non-toxic, but it also recycles organic waste, consistent with the green chemistry principles. CuNPs synthesized were then primarily characterized through Dynamic Light Scattering (DLS) and UV-Vis spectroscopy, confirming the production of nano-scaled particles with good dispersibility. The average particle size determined by DLS is around 35-40 nm.

The use of CuNPs showed high affinity with the fingerprint residue-made primarily from sweat, amino acids, as well as naturally excreted human skin oil in the development of latent prints in both porous (paper) and non-porous surfaces (metal knife). The results of the present research demonstrate notable visualization of latent fingerprint development as compared to traditional black powder. This process enhanced the contrast of the details in the ridges to yield high-contrast prints. The green method reduces chemical waste and health hazards found in standard approaches by providing an affordable, sustainable solution for nanomaterial production. Further studies will evaluate the function of biosynthesized CuNPs across different surfaces in terms of sensitivity and stability.

---

**KEYWORDS:** Advanced nanomaterials, Green synthesis, Forensic nanotechnology application, Latent fingerprint detection, Nanotechnology in life sciences

---

**ACKNOWLEDGEMENTS:** Our sincere thanks to Amity University Dubai for providing the opportunity and resources to acquire firsthand learning and work experience.

---

### REFERENCES

- [1] S.A. Sari, U. Qalbiah, I.C. Putri, “Comparison between latent fingerprint identification using black powder and cyanoacrylate glue”, *Asian. J. Chem.* 30:2615-2620 (2018).
- [2] R. Rohatgi, F. Dominica, “Application of Nanotechnology in Forensic Science”, *J. Forensic Sci.* (2022). <https://doi.org/10.37421/2157-7145.2022.13.507>
- [3] H. Huang, J.J. Lv, D.L. Zhou, N. Bao, Y. Xu, A.J. Wang, J.J. Feng, “One-pot green synthesis of nitrogen-doped carbon nanoparticles as fluorescent probes for mercury ions,” *R.S.C. Adv.* 3:21691-21696 (2013). <https://doi.org/10.1039/C3RA43452D>

## Plasma-assisted synthesis of PLA-derived nanoparticles with tunable structure

K. Skorvankova<sup>1</sup>\*, J. Štátná<sup>1</sup>, D. Nikitin<sup>1</sup>, I. Křivka<sup>1</sup>, I. Krakovský<sup>1</sup>, Z. Krtouš<sup>1</sup>, J. Kousal<sup>1</sup>, P. Solař<sup>1</sup>

*1) Charles University, Faculty of Mathematics and Physics, V Holešovičkách 2, 180 00 Prague 8, Czech Republic, Czech Republic*

\* katerina.skorvankova AT matfyz.cuni.cz

This work introduces a dry physical approach for the synthesis of polymer-derived nanoparticles from a poly(lactic acid) (PLA) precursor using a gas aggregation source (GAS) combined with plasma-assisted vacuum thermal deposition (PAVTD). In this filament-fed system, a polymeric filament is continuously supplied and thermally evaporated into the aggregation chamber. Unlike magnetron sputtering or plasma-enhanced chemical vapor deposition (PECVD), this approach enables nanoparticle formation from polymer-like fragments, allowing partial preservation of the original polymer structure. Vaporized species undergo fragmentation and repolymerization under plasma conditions, forming nanoparticles that are subsequently transported through an orifice for deposition.

The structure of the nanoparticles is strongly influenced by deposition parameters. Preliminary results indicate that increasing plasma power leads to a progressive loss of the original PLA backbone and promotes the formation of more cross-linked plasma-polymer nanostructures. These structural and chemical changes are characterized using SEM, XPS, FTIR, NMR, and GPC.

The integration of continuous filament feeding, together with feedback control of the evaporation rate, improves process stability and reproducibility compared to conventional PAVTD approaches. The presented method offers a promising route for the controlled synthesis of polymer-based nanoparticles with tunable chemical structure.

---

**KEYWORDS:** Plasma-Assisted deposition, Plasma-polymers, Gas aggregation source

---

**ACKNOWLEDGEMENTS:** This work was supported by The Czech Science Foundation (GACR) under grant No. 25-15644S.

## Carbon dots from torrefied wheat bran obtained by NaOH exfoliation - properties, calcium modification and fluorescence detection

W. Matyjasik<sup>1\*</sup>, M. Banach<sup>2</sup>

1) Cracow University of Technology, Faculty of Chemical Engineering and Technology, Department of Chemical Technology and Environmental Analytics, 31-155 Krakow, Poland, Poland

2) Faculty of Chemical Engineering and Technology, Cracow University of Technology, Cracow, Poland

\* matyjasik.wiktoria.96 AT gmail.com

Carbon dots (CDs) are versatile 0D carbon nanostructures whose optical properties strongly depends on the core structure and surface chemistry. They are promising fluorescent nanomaterials; however, sustainable synthesis routes are still needed. Here, we present a modified top-down method to produce CDs from wheat bran by combining mild pyrolysis (220-400°C, 10-60 min) with aqueous NaOH exfoliation, followed by neutralization and multistage purification (filtration and dialysis). The influence of thermal treatment on structure and optical properties was assessed using FT-IR, XRD, and HR-TEM, together with UV-Vis and fluorescence spectroscopy. We investigated correlations between processing conditions, nanostructure, and photoluminescence. CDs obtained at 400°C for 60 min (WB-400-60) were highly crystalline and showed a narrow size distribution (~2.7 nm). They exhibited a fluorescence quantum yield of 17.1% at an excitation wavelength of 290 nm. The UV emission was stable, with an emission maximum at ~334 nm upon excitation in the 250-300 nm range. Calcium acetate modification (WB-400-60-Ca) changed the fluorescence characteristics: the excitation maximum shifted (from 290 to 310 nm) and the excitation-independent emission range broadened (to ~250-350 nm), with an emission maximum at ~410 nm. The CDs were evaluated as fluorescent probes, and optical detection was based on fluorescence quenching. The WB-400-60 CDs were used for the determination of Fe<sup>2+</sup> (0.5-50 µM; LOD 74.1 nM), chloridazon (0.01-10 mg/L; LOD 0.35 µM), and paracetamol (1-40 mg/L; LOD 0.5 µM). These results confirm that waste biomass such as wheat bran is a viable precursor for functional CDs and that metal-ion modification can be used to alter their optical response; future work will focus on more controlled modification with metal cations to further tune emission and selectivity.

---

**KEYWORDS:** Carbon dots, Chemical exfoliation, Biomass-derived nanomaterials, Calcium modification, Optical detection

---

**ACKNOWLEDGEMENTS:** This work was carried out as part of the research project No. 2025/57/N/ST5/04585 funded by the National Science Centre, Poland.

## Squid cartilage-derived carbon quantum dots for selective fluorescence sensing of hexavalent chromium in water

A. Sobti<sup>1</sup>\*

1) Dubai College, United Arab Emirates

\* abhisobti100 AT gmail.com

The detection of hexavalent chromium in water remains a significant analytical challenge due to its high toxicity, widespread industrial origin and high solubility, which facilitates rapid dispersion in aquatic systems. In the present study, carbon quantum dots (CQDs) were synthesized through a hydrothermal process using squid cartilage derived from *Uroteuthis duvaucelii*. This marine biowaste material has not been previously explored for such applications. The resulting squid cartilage-derived CQDs (SC-CQDs) exhibit an average particle size of 4.28 nm and are readily dispersible in aqueous media. Microscopic and spectroscopic characterisations reveal the formation of nanoscale carbon frameworks enriched with oxygenated surface functionalities, which play a crucial role in the observed optical behaviour. The SC-CQDs exhibit excitation-dependent photoluminescence, along with a measurable dependence on solution pH, indicating the contribution of surface states to their emission. Their sensing performance of SC-CQDs was systematically evaluated against various metal ions, among which Cr(VI) induced a pronounced selective quenching of fluorescence intensity. A concentration-dependent response was obtained, yielding a limit of detection of 5.4  $\mu\text{M}$ . Although the sensing performance does not surpass that of highly sophisticated analytical platforms, the simplicity of synthesis, low material cost, and operational ease render the SC-CQDs particularly suitable for preliminary monitoring of chromium contamination in resource-limited and minimally equipped settings. Overall, this study demonstrates the viability of SC-CQDs as sustainable and efficient fluorometric probes for chromium detection in aqueous environments.

**KEYWORDS:** Carbon quantum dots, Squid cartilage (*Uroteuthis duvaucelii*), Hydrothermal synthesis, Photoluminescence quenching, Hexavalent chromium (Cr(VI)) sensing

### REFERENCES

- [1] J. Kotas and Z. Stasicka, "Chromium occurrence in the environment and methods of its speciation," *Environmental Pollution*, 2000.
- [2] M. Costa, "Potential hazards of hexavalent chromate in our drinking water," *Toxicology and Applied Pharmacology*, 2003.
- [3] J. Wang *et al.*, "Detection methods for chromium species in environmental samples," 2017.
- [4] Z. Zhu *et al.*, "Fluorescence-based sensing approaches for heavy metal detection," 2015.
- [5] S. N. Baker and G. A. Baker, "Luminescent carbon nanodots," *Angewandte Chemie*, 2010.

## Mefenamic acid-stabilized silver nanoparticles act as nano-elicitors to enhance callus biomass and antioxidant metabolism in *Moringa oleifera* in vitro

N. Anwar<sup>1\*</sup>, Z. Akbar<sup>1</sup>, M. Rauf<sup>2</sup>, M. Arif<sup>1</sup>, A. Ullah<sup>1</sup>, S. H. Anwar<sup>3</sup>, R. Shah<sup>1</sup>, M. Shah<sup>1</sup>, S. Azizi<sup>4</sup>

1) Abdul Wali Khan University Mardan, Pakistan

3) Bacha Khan University Charsada, Pakistan

4) UNESCO-UNISA Africa Chair in Nanosciences/Nanotechnology, College of Graduate Studies, University of South Africa, Muckleneuk Ridge, Pretoria, South Africa., South Africa

\* natasha AT awkum.edu.pk

Nanotechnology has become a potent means in plant biotechnology field as it offers new methods to control growth, metabolism and stress responses in in vitro environment. In this paper, we report the synthesis of mefenamic acid-stabilized silver nanoparticles (MA-AgNPs) by a chemical reduction technique and determine their nano-elicitor activity in *Moringa oleifera* callus cultures. The nanoparticles were characterized by UV-visible spectroscopy, Fourier-transform infrared spectroscopy, scanning and transmission electron microscopy, and X-ray diffraction. The characterization confirmed the formation of crystalline, face-centered cubic (fcc) silver nanoparticles with mostly spherical morphology and an average particle size of about 27 nm, which demonstrates that mefenamic acid was effective in stabilising the nanoparticles.

The influence of MA-AgNPs on biomass production and metabolic responses was obtained by treating callus cultures with MA-AgNPs at 10-100 ppm. The supplementation of MA-AgNP had a strong positive impact on growth of the callus in comparison with untreated controls, and the callus reached maximum fresh biomass (22.61 g per culture) at the concentration of 100 ppm. Additionally, it boosted secondary metabolite production such as total phenolics (2.46mg GAE g-1FW), total flavonoids (3.68mg QE g-1FW) under AgNP treatment.

It was also observed that there was a high level of antioxidant defense mechanism stimulation which was determined by high levels of glutathione (139.75  $\mu\text{g g}^{-1}$  FW), presence of superoxide dismutase (53.78 U mL<sup>-1</sup> protein), presence of ferric reducing antioxidant power (54 mg AAE g<sup>-1</sup> FW), and presence of DPPH radical scavenging activity (76.3%). On the whole, these findings suggest that MA-AgNPs are effective nano-elicitor, in the stimulation of callus biomass formation and antioxidant metabolites biosynthesis in *M. oleifera*.

---

**KEYWORDS:** *Moringa oleifera*, Silver nanoparticles, Mefenamic acid, Callus culture, Secondary metabolites

---

**ACKNOWLEDGEMENTS:** Funding: This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

---

### REFERENCES

- [1] R. Balachandar, *et al.*, Antibacterial activity of silver nanoparticles phytosynthesized from *Glochidion candolleianum* leaves. *Materials Letters*, 2022. 311: p. 131572.
- [2] M. Sharma, *et al.*, A Brief Review of Plant Cell Transfection, Gene Transcript Expression, and Genotypic Integration for Enhancing Compound Production. *Gene, Drug, and Tissue Engineering*, 2023: p. 153-179.
- [3] S. Asad, *et al.*, Biological synthesis of silver nanoparticles by *Amaryllis vittata* (L.) Herit: from antimicrobial to biomedical applications. 2022. 15(16): p. 5478.
- [4] N. Mohammadkhani, R.J.W.A.S.J. Heidari, Drought-induced accumulation of soluble sugars and proline in two maize varieties. 2008. 3(3): p. 448-453.
- [5] E.J.J.A.M. Van C.A. Handel, Rapid determination of glycogen and sugars in mosquitoes. 1985. 1(3): p. 299-301.

Posters

T1-19

E-POSTER

**Synthesis and characterization of EuFeO<sub>3</sub> nanopowders with a perovskite-type structure**

O. Chudinovych<sup>1\*</sup>, S. Korichev<sup>2</sup>, V. Kolesnichenko<sup>1</sup>, D. Vedel<sup>1</sup>

1) Frantsevich Institute for Problems of Materials Science, NAS of Ukraine, Ukraine

2) Frantsevich Institute for Problems of Material Science, NAS of Ukraine, Ukraine

\* olgachudinovych AT gmail.com

Orthoferrites of rare-earth elements RFeO<sub>3</sub> (R = rare-earth ion) have been the subject of intensive research due to their electrical and magnetic properties, which are determined by the interaction between spin, orbital, and crystal-chemical degrees of freedom. RFeO<sub>3</sub> also exhibits high thermal stability and electrical conductivity, low dielectric losses, high dielectric permittivity, ferroelectricity, polarizability, etc. [1-2].

The nanocomposites were obtained by the Pechini method and the heterogeneous precipitation method. Solutions of Eu<sup>3+</sup> nitrates, obtained by dissolving europium oxides with a main-component content of 99.99% in nitric acid, were used as starting materials. Mixtures with different Fe<sup>3+</sup> contents were prepared from nitrate solutions. The obtained precursor was dried at 120 °C for 24 hours and then subjected to heat treatment at 800 °C. The characteristics of the samples were determined using physicochemical methods: X-ray diffraction (XRD), thermogravimetric (TG) and differential thermal (DTA) analysis, and electron microscopy. The nanocomposites were identified as having a perovskite-type structure. The XRD patterns do not show any other peaks corresponding to Eu, Fe, Eu<sub>2</sub>O<sub>3</sub>, Fe<sub>2</sub>O<sub>3</sub>, or any other additional impurity-related phases. According to SEM, the synthesized powders have a conglomerate structure. EuFeO<sub>3</sub> exhibits a granular nanocrystalline microstructure composed of nearly isometric, rounded particles with typical sizes of 60-125 nm.

The EuFeO<sub>3</sub> samples, characterized by a predominantly isometric granular microstructure and dense nanoparticle agglomeration, exhibit relatively low specific surface areas of 2.49 and 7.61 mZ/g. This morphology results in a compact structure, which is reflected in lower densities of 6.46 and 6.87 g/cm<sup>3</sup>. The negative ζ-potential value of -14 mV indicates limited electrostatic stability of the particles in the dispersed medium and their tendency toward agglomeration, which is consistent with the observed compact microstructure.

**KEYWORDS:** EuFeO<sub>3</sub> nanopowders, Orthoferrites, Perovskite structure, Pechini method, Rare-earth ferrites

**REFERENCES**

- [1] R.L. White. Review of recent work on the magnetic and spectroscopic properties of the rare-earth orthoferrites // J. Appl. Physics, 40 (1969) 1061-1069.
- [2] P. K. Pradhan, A.B. Panda, G.K. Mishra, N.K. Mohanty. Rare earth orthoferrites (RFeO<sub>3</sub>, R = rare earth elements): A comprehensive review of structural, dielectric, and magnetic properties // Smart Mater. Manuf., 3(2025) 100082.

## Photocatalytic activity of the heterostructures based on $\text{CeO}_2\text{-La}_2\text{O}_3\text{-Dy}_2\text{O}_3$ fluorite and anatase

O. M. Lavrynenko<sup>1</sup>\*, M. Z. Mykitovich<sup>2</sup>, A. Ragulya<sup>3</sup>, S. Korichev<sup>4</sup>

1) I.M. Frantsevich Institute for Problems of Material Science of National Academy of Science of Ukraine, Ukraine

2) I.M. Francevich Institute for Problems of Materials Science NAS of Ukraine, Ukraine

3) Frantsevich Institute for Problems of Materials Science of NAS of Ukraine, Ukraine

4) Frantsevich Institute for Problems of Material Science, NAS of Ukraine, Ukraine

\* alena.lavrynenko AT gmail.com

Today, progress in the development of photocatalytic materials for ‘green’ technologies and environmental protection is focused on improving the optical properties of semiconductor oxides and creating composite structures based on them. One effective strategy for improving the optical characteristics of titanium dioxide is to create heterostructures based on it by introducing cerium dioxide and other rare-earth elements into its composition, which can contribute both to improving the photocatalytic activity of the photocatalyst and to increasing its stability in aggressive environments and extending its service life. In our study, a new heterostructure based on cerium, lanthanum, and dysprosium was created, with an anatase component (CSR = 11.5 nm). The heterostructures were formed by mechanosynthesis, followed by thermal treatment of the powder to ensure heterojunctions between the components of the nanocomposite system.

The photocatalytic activity of the samples was tested using solutions of methylene blue (MB), rhodamine B (RhB), methyl orange (MO), and orange G (OG) with initial dye concentrations of 20 mg/dm<sup>3</sup>. The experiments and calculations of the parameters were carried out according to standard methods. The data obtained show that the presence of dysprosium in the structure of the samples inhibits the photocatalytic decomposition of cationic dyes, whereas in the presence of  $\text{CeO}_2$  (95 mol.%)- $\text{La}_2\text{O}_3$  (5 mol.%)- $\text{TiO}_2$  particles, photodegradation of MB and RhB occurs. At the same time, the molecules of the anionic dyes OG and MO interact intensively with the surface of the heterostructures and decompose over time. The reaction rate constants are in the range of  $10^{-3}$  to  $10^{-4}$ . Thus, the introduction of a titanium-containing component allows the activity of the rare-earth fluorite to be shifted from the visible light region to the UV region.

---

**KEYWORDS:** Photocatalysis,  $\text{TiO}_2$  heterostructures, Cerium dioxide, Rare-earth oxides, Semiconductor oxides

## Quinoline derivatives as fluorescent probes for zinc determination in living cells

M. Yeshchenko<sup>1\*</sup>, P. Virych<sup>2</sup>, P. Virych<sup>3</sup>, V. Smokal<sup>3</sup>, N. Kutsevol<sup>2</sup>

1) Faculty of Chemistry, Taras Shevchenko National University of Kyiv, Ukraine

2) Taras Shevchenko National University of Kyiv, Ukraine

3) Chemical Faculty, Taras Shevchenko National University of Kyiv, Ukraine

\* m.yes1410 AT gmail.com

$\text{Ca}^{2+}$ ,  $\text{Mg}^{2+}$ , and  $\text{Zn}^{2+}$  are the most abundant divalent cations in the body. 8-Hydroxyquinoline (8HQ) are known for its wide range of optical, chemical properties and biological effects. Cation chelation is an important feature of these compounds in the creation of biologically active substances. Metal complexes of 8HQ exhibit antibacterial and antiproliferative activity. 8HQ derivatives possess favorable photophysical and coordination properties for developing fluorescent metal sensors. N-(6-methoxy-8-quinoliny)-4-methylenebenzenesulfonamide (TSQ) is well known as a fluorescent indicator of intracellular zinc. The aim was to determine the possibilities of chelation of calcium, magnesium and zinc by (8HQ) derivatives 2-(4-methoxystyryl)quinolin-8-ol (STQ-Me), 2-(4-ethoxyphenylethenyl) quinolin-8-ol (STQ-Et) and 2-(4-(trifluoromethyl)styryl)quinolin-8-ol (STQ-CF<sub>3</sub>) based on physiological solution. The potential of this substance for studying dynamic changes in intracellular zinc was tested in comparison with the TSQ. The cytotoxicity and fluorescence of test molecules in living cells in the presence of cations was investigated.

To assess the potential use of 8HQ derivatives as fluorescent indicators for zinc detection, a model involving loading KB cells with ZnO nanoparticles (NPs) was selected. When using TSQ, a statistically significant increase in intracellular zinc levels was observed after 30 minutes of incubation with ZnO NPs. The maximum values of the indicator were reached after 45 min and remained stable at this level for up to 2 h. The baseline integrated density of KB cells after staining with TSQ was 25 200 a.u. (median). The baseline integral density of KB cells after staining with STQ-Me was 9 800 a.u., which was 2.5 times less than similar indicators for TSQ. The maximum level of cell fluorescence was recorded after 30 min of incubation. No significant changes in baseline fluorescence of KB cells were observed after STQ-Et staining. Fluorescence increased after 15 min of incubation and began to be restored after 30 min. No changes in cell fluorescence were identified after STQ-CF<sub>3</sub> using. Fluorescent aggregates of STQ-CF<sub>3</sub> were identified between cells. No significant cytotoxicity of the investigated compounds was found.

Based on the results, the 8HQ derivatives STQ-Et and STQ-CF<sub>3</sub> were found unsuitable for assessing zinc levels in living cells. STQ-Me shows potential for measuring zinc levels in living cells. However, STQ-Me was most likely not able to chelate protein-bound zinc, as evidenced by the dynamic fluorescence parameters of KB cells. Thus, STQ-Me has the potential for use in measuring zinc in living cells, but the molecular design requires modification to enhance fluorescence and expand its ability to chelate protein-bound zinc.

---

**KEYWORDS:** 8-Hydroxyquinolines, Zinc sensing, ZnO nanoparticles, Fluorescent probe

## Synthesis of titanium matrix composites reinforced with TiB nanosized particles

V. Nevmerzhytskyi<sup>1</sup>, D. Vedel<sup>2</sup>, O. Stasiuk<sup>1\*</sup>

1) G. V. Kurdyumov Institute for Metal Physics of the N.A.S. of Ukraine, Ukraine

2) Frantsevich Institute for Problems of Materials Science, NAS of Ukraine, Ukraine

\* olek.stasiuk AT gmail.com

Titanium alloys are widely recognized as advanced structural materials due to their unique combination of high specific strength, excellent corrosion resistance, and relatively low density. These properties enable their extensive application in aerospace, marine, biomedical, and defense industries, where weight reduction and high mechanical performance are critical requirements. In particular, titanium alloys retain high strength over a wide temperature range and demonstrate superior resistance to aggressive environments, making them suitable for demanding operating conditions. Consequently, further enhancement of their mechanical properties, especially hardness and strength, remains an important scientific and technological challenge.

In this work, titanium matrix composites reinforced with nanosized titanium monoboride (TiB) particles were synthesized using a TiH<sub>2</sub>-TiB<sub>2</sub> powder system. The formation of TiB occurs in situ due to boron diffusion from TiB<sub>2</sub> into the titanium matrix, which ensures strong interfacial bonding and the absence of macrodefects at phase boundaries. The synthesis process leads to the formation of TiB particles with a characteristic needle-like morphology.

It was established that the growth of TiB needles is anisotropic and controlled by preferential boron diffusion along the [010] crystallographic direction. As a result, high aspect ratio nanosized reinforcements are formed. The size and distribution of TiB needles can be effectively controlled by adjusting the synthesis temperature and holding time.

The introduction of nanosized TiB needles significantly improves mechanical properties of the composites, including tensile strength, hardness, and elastic modulus. An increase in the reinforcing phase content above 3 wt.% results in further strengthening; however, a reduction in plasticity is observed. Despite a slight increase in residual porosity, the overall mechanical performance is enhanced due to effective load transfer and reinforcement mechanisms.

The proposed approach can also be applied to the fabrication of irregularly shaped titanium powders reinforced with nanosized TiB, which are promising for additive manufacturing applications.

---

**KEYWORDS:** Titanium matrix composites, TiB reinforcement, Nanosized particles, In situ synthesis, Titanium diboride

---

**ACKNOWLEDGEMENTS:** This work was supported by the National Academy of Sciences of Ukraine under the program “Grants of the NAS of Ukraine for Research Laboratories/Groups of Young Scientists” (registration number 0126U002256).

## Optimization of the composition and content of composite carbon filler in rubber compositions using different formulations

Y. Sementsov<sup>1, 2 \*</sup>, Z. Dong<sup>3</sup>, M. Wu<sup>1</sup>, K. Ivanenko<sup>4, 1</sup>, Y. Hrebelsna<sup>5</sup>, D. Wang<sup>3</sup>, S. Hozhdzinskiy<sup>6</sup>,  
S. Makhno<sup>1, 2</sup>, K. Sencha-Hlevatska<sup>2</sup>, M. Terets<sup>2</sup>, O. Ihnatenko<sup>2</sup>, M. Kartel<sup>2</sup>

1) Ningbo Sino-Ukrainian New Materials Industrial Technologies Institute; Ningbo University of Technology, China

2) Chuiko Institute of Surface Chemistry of National Academy of Sciences of Ukraine, Ukraine

3) Ningbo University of Technology, China

4) Institute of Macromolecular Chemistry of National Academy of Sciences of Ukraine, Ukraine

5) TMSpetsmash Ltd, Ukraine

6) Bogomolets National Medical University, Ukraine

\* ysementsov AT ukr.net

Today, there are many optimized multi-component (up to 12-18) rubber compositions, the characteristics of which can be improved by using modern achievements of nanotechnology - nanosized carbon fillers. The biggest problem of using hybrid (composite) fillers, traditional carbon black (CB) in a composition with nanosized carbon materials, for example, carbon nanotubes (CNTs), is achieving a homogeneous distribution of fillers, as a result of the sequential mixing of several components in the matrix. The probability of homogeneous distribution decreases with increasing number of fillers, as does the probability of simultaneous occurrence of interdependent processes, i.e. it is equal to the product of individual probabilities.

The solution to this problem involves the creation of uniformly distributed CB@CNT fillers during CB synthesis (by introducing CNTs into hydrocarbon (CH) raw materials (HCRM), in-situ), which are then added into the rubber matrix, and the ratio of the amounts of CNTs and HCRM, as well as the CB@CNT content in the rubber composition, are pre-calculated.

We assume that to create a solid non-porous rubber composition (we consider the content of CB to be already optimized by the method of sorting out the options), the rubber must wet the entire filler system, creating a layer with a thickness equal to two average diameters of CNTs ( $d_{CNT}$ ). And the content of CB in the rubber composition according to the initial recipe is reduced by the mass of CNTs in proportion to the ratio of the specific surfaces of CB and CNTs.

That is:  $V_{RUB}/(S_{CB} \times m_{CB} + S_{CNT} \times m_{CNT}) = 2d_{CNT}$  (1),

where:  $V_{RUB}$  - volume of rubber;  $S_{CB}$  - specific surface area of CB;  $m_{CB}$  - mass fraction of carbon nanotubes;

$S_{CNT}$  - specific surface area of CNT;  $m_{CNT}$  - mass fraction of CNTs; and  $m_{CB} = m_{CB}^0 - (S_{CB}/S_{CNT}) \times m_{CNT}$  (2)

where:  $m_{CB}^0$  - mass fraction of CB in the rubber composition according to the original recipe. After simple

transformations of the system of equations (1) and (2), we obtain the determination of the ratio of the masses of CNT and HCRM:  $m_{CNT}/m_{CH} = K \times (\alpha - 2\rho_{RUB} \times S_{CB} \times d_{CNT}) / \{2\rho_{RUB} \times d_{CNT} \times S_{CNT} [1 - (S_{CB}/S_{CNT})^2]\}$  (3), where:

$K = m_{CB}/m_{CH}$  - CB output ratio,  $\alpha = m_{RUB}/m_{CB}^0$  and  $m_{CB}^0 = K \times m_{CH}$ . And, the content of the composite filler in

the rubber composition, in phr of rubber:  $m_{CB+CNT} = m_{CB}^0 \times \{1 + (\alpha - 2\rho_{RUB} \times S_{CB} \times d_{CNT}) \times (1 - S_{CB}/S_{CNT}) / (2\rho_{RUB} \times d_{CNT} \times S_{CNT} \times [1 - (S_{CB}/S_{CNT})^2])\}$  (4)

The calculated ratios of CNTs and HCRM and the content of the composite filler were used for the synthesis of the composite filler CB@CNT and the production of rubber compositions based on synthetic rubber NBR 3365 and natural rubbers SMR and SMR 20. The determined mechanical characteristics showed their increase in the series from the CB filler, the calculated content of mixtures of CB and CNTs and composite CB@CNT for all three systems and in comparison, with analogues. This shows the correctness of the assumptions made and the effectiveness of the use of CB@CNT synthesis in situ mode.

**KEYWORDS:** Rubber composition, Carbon black, Carbon nanotubes, Nanosized carbon fillers, Hydrocarbon raw materials

**ACKNOWLEDGEMENTS:** This research was funded by the National Key R&D Program of China-Strategic Collaboration Key Project 2023YFE0201200. This paper is sponsored by the Ningbo Sino-Ukrainian New Materials Industrial Technologies Institute Co, Ltd.

## The electrophysical and mechanical properties relationship of epoxy-based fiberglass composites with carbon nanotubes

S. Makhno<sup>1, 2</sup>, O. Lisova<sup>2</sup>, P. Gorbyk<sup>2</sup>, D. Wang<sup>3</sup>, Z. Dong<sup>3</sup>, H. Tang<sup>4</sup>, H. Potapenko<sup>5</sup>, K. Ivanenko<sup>6, 1 \*</sup>,  
Y. Sementsov<sup>1, 2</sup>

1) Ningbo Sino-Ukrainian New Materials Industrial Technologies Institute; Ningbo University of Technology, China

2) Chuiko Institute of Surface Chemistry of National Academy of Sciences of Ukraine, Ukraine

3) Ningbo University of Technology, China

4) AGH University of Science and Technology, China

5) V.I. Vernadsky Institute of General and Inorganic Chemistry of the NAS of Ukraine, Ukraine

6) Institute of Macromolecular Chemistry of National Academy of Sciences of Ukraine, Ukraine

\* k\_ivanenko AT i.ua

Products made from electrically conductive fiberglass are widely used as electromagnetic shields and antistatic coatings. The functional fillers of such materials include special grades of carbon black, graphite, carbon fibers. Particular attention is paid to the use of carbon nanotubes (CNTs), which are characterized by high conductivity and enhanced mechanical strength. The aim of this work was to investigate the electrophysical and mechanical properties of fiberglass plastics based on epoxy resin (ER) with varying CNT content in different regions of the samples.

To form the composites, four layers of ST-48 glass fabric, EPOLAM 5015 RESIN epoxy resin were used. The CNTs were dispersed using a three-roll mill, with CNT concentrations ranging from 0 to 0.5% in the polymer. Samples of size 150×150×1.5 mm were formed by infusion pressing. Measurements of conductivity were carried out using alternating current in the frequency range to 100 kHz using the two-contact method. The mechanical properties of the fiberglass plastics were determined under tension using an R-50 tensile testing machine.

The non-linear behavior of conductivity with respect to CNT content indicates the presence of a percolation transition in the system at approximately 0.1% (0.0006 volume fraction). For composites with a CNT content of up to 0.25% (2.5 times the percolation threshold), an increase in tensile strength values is observed; with a further increase in content, the tensile strength decreases while the conductivity increases. In the content range of 0.3-0.5% (significantly exceeding the percolation threshold), the tensile strength decreases due to a reduction in the specific adhesion of the polymer to the CNTs (insufficient liquid polymer surface to wet the CNTs, resulting in increased porosity). At the optimal CNT content, the tensile strength exceeds that of composites without CNTs by more than 1.6 times.

Analysis of the electrophysical characteristics of composites indicates a significant difference in their properties across different regions. The highest values of conductivity are observed in the central parts of the fiberglass plastics, as are the highest values of tensile strength. Lower values at the periphery of the samples (by approximately 10%) are due to the orientation and filtration of CNTs during composite formation. At the same CNT content, the flexural strength is higher for sample regions that have higher electrical conductivity, provided the CNT content is less than 2.5 percolation thresholds. It has been shown that up to a CNT content of 2.5 times the percolation threshold, both conductivity and tensile strength increase; with a further increase in CNT content, electrical conductivity increases while tensile strength decreases. The decrease in tensile strength upon addition of carbon nanotubes, equal to 2.5 percolation thresholds, is associated with a decrease in the specific adhesion surface area during wetting of carbon nanotubes with polymer

---

**KEYWORDS:** Carbon nanotubes, Conductivity, Fiberglass, Epoxy resin, Mechanical properties

---

**ACKNOWLEDGEMENTS:** This paper is sponsored by the Ningbo Sino-Ukrainian New Materials Industrial Technologies Institute Co, Ltd.

## Decoration of copper foam with silver nanostructures by galvanic replacement

V. Skrypnychuk<sup>1</sup>\*, V. Hreb<sup>1</sup>, G. Zozulya<sup>1</sup>, E. Matsko<sup>1</sup>, O. Kuntiyi<sup>1</sup>

*1) Lviv Polytechnic National University, Ukraine*

\* skrypnychuk AT gmail.com

The oxygen reduction reaction (ORR) is one of the processes that limits the application of fuel cells and secondary metal-air batteries. The main reason for this is the insufficient efficiency of existing electrocatalysts. The most active among them, based on platinum, are hindered in scalability due to the high cost and limited natural resources of this metal. Therefore, research aimed at finding non-platinum ORR electrocatalysts is highly relevant. One alternative is cathodes based on significantly cheaper silver, which is second only to platinum and palladium in terms of O<sub>2</sub> binding energy. Emphasis is placed on nanostructures, bimetallic systems, and high specific surface area [1].

In this work, the possibility of forming catalytically active ORR cathodes (Ag/Cu<sub>foam</sub>) based on silver nanostructures deposited on the surface of commercial copper foam by the galvanic replacement method is demonstrated. The latter is effective for depositing metal nanostructures onto the surface of 3D sacrificial metals [2, 3]. Silver was deposited from solutions of (1) AgNO<sub>3</sub> and (2) ammine complexes [Ag(NH<sub>3</sub>)<sub>2</sub>]<sup>+</sup>. It is shown that in the first case, the formation of discrete nanoparticles (<50 nm) and dendrites is typical, while in the second case, structures range from nanoparticles (<20 nm) and their agglomerates to porous nanofilms. A relatively uniform distribution of the silver deposit over the entire surface of the copper foam is observed. The main parameters influencing the geometry of the deposited nanoparticles and the degree of surface coverage with silver are the concentration of hydrated and complex ions and the duration of galvanic replacement. A dependence of electrochemical ORR activity measured using the obtained Ag/Cu<sub>foam</sub> cathodes on the morphology of the nanostructured surface has been established. The synergistic effect of the Ag-Cu bimetallic system and the positive impact of a large specific surface area are demonstrated.

---

**KEYWORDS:** Electrochemistry, Electrocatalysis, Oxygen reduction reaction, Galvanic substitution, Silver nanoparticles

---

**ACKNOWLEDGEMENTS:** This work was carried out with the partial financial support of the National Research Foundation of Ukraine. Project registration number: 2025.07/0068 (“Bimetallic nanostructures formed via laser treatment and decoration of 3D substrates by galvanic replacement in electrochemical catalysis: design, architecture of electrodes, topography, activity, stability”).

---

### REFERENCES

- [1] O. Kuntiyi, V. Skrypnychuk, and H. Zozula, “O<sub>2</sub> Electroreduction on Silver and Silver-Based Nanostructured Cathodes: A Review,” *Int. J. Energy Res.*, 2481690, 2025.
- [2] A. G. M Da Silva, T. S. Rodrigues, S. J. Haigh, and P. H. C. Camargo, “Galvanic replacement reaction: recent developments for engineering metal nanostructures towards catalytic applications,” *Chem. Commun.*, vol. 53, pp. 7135-7148, 2017.
- [3] R. Thota, S. Sundari, S. Berchmans, and V. Ganesh, “Silver - Copper Bimetallic Flexible Electrodes Prepared Using a Galvanic Replacement Reaction and Their Applications,” *ChemistrySelect*, vol. 2, pp. 2114-2122, 2017.

## Formation and confinement of nanoparticles in a mid-frequency rectangular-wave discharge

V. Lisovskiy<sup>1</sup>\*, S. Dudin<sup>1</sup>, S. Bogatyrenko<sup>1</sup>, S. Rezunenko<sup>1</sup>

1) V.N. Karazin Kharkiv National University, Kharkiv, Ukraine

\* lisovskiy AT yahoo.com

Nanoparticles (NPs) synthesized in acetylene plasma are of interest not only from a fundamental perspective but are also considered promising carriers of antibiotics for targeted delivery. In most studies reported in the literature, experiments are performed with horizontally aligned electrodes, and the formed NPs are confined within the discharge volume by high electric fields of the near-electrode regions, either in RF capacitive discharges or in the cathode sheath of DC glow discharges.

We investigate NPs formation in a bipolar mid-frequency rectangular-wave discharge, where the discharge tube is oriented horizontally while the electrodes are mounted vertically. The inner diameter of the tube is 80 mm, and the distance between the plane electrodes is 76.2 mm. NPs formed in the plasma were deposited both on a glass slide for optical microscopy placed at the bottom of the tube and on separate TEM support grids positioned on the same slide. Bipolar rectangular-wave voltage with peak-to-peak amplitude up to 1300 V and frequencies in the range of 17-200 kHz were applied to one of the electrodes. Acetylene was introduced into the discharge chamber with the pressure in the range of 0.05-1 Torr.

Since the NPs are too small to be directly observed with the naked eye, laser light scattering diagnostics were employed. The laser beam was expanded into a flat light sheet using a cylindrical lens. This approach enabled visualization of 2D cross-sections of the NPs cloud, while scanning the light sheet allowed reconstruction of its 3D structure.

In DC glow discharge, the NPs cloud is typically narrow and localized within the negative glow region, confined by a potential well. In contrast, in the bipolar mid-frequency rectangular-wave discharge, the NPs cloud was found to be significantly broader. During the positive phase of the voltage pulse, the driven electrode acts as an instantaneous anode, while the opposite electrode serves as an instantaneous cathode; during the negative phase, their roles are reversed. Electrons and positive ions rapidly respond to the alternating electric field. However, negatively charged NPs, due to their large mass and inertia, respond primarily to the time-averaged electric field. The spatial distribution of the time-averaged potential exhibits a maximum between the boundaries of two cathode sheaths formed near the instantaneous cathodes. Consequently, a wide potential well is established in this region, enabling both formation and long-term confinement of NPs, which was confirmed experimentally. The width of the potential well, and correspondingly the NPs cloud, increases with decreasing pulse frequency and increasing peak-to-peak voltage.

Transmission electron microscopy revealed that the NPs are predominantly spherical with diameters of 100-200 nm. They are rarely isolated; instead, they tend to form elongated chains of complex morphology, often assembling into fractal-like agglomerates with sizes of several micrometers.

---

**KEYWORDS:** DC glow discharge, Acetylene, Formation and confinement of nanoparticles, Potential well

## SECM-assisted polishing of carbon nanoelectrodes for high-resolution electrochemical mapping

V. Shrivastav<sup>1</sup>\*, D. Disha<sup>1</sup>, V. Shrivastav<sup>2</sup>, W. Nogala<sup>1</sup>

1) Institute of Physical Chemistry Polish Academy of Sciences, Poland

2) Regional Centre of Advanced Technologies and Materials, Czech Advanced Technology and Research Institute, Palacký University, Olomouc, Czech Republic

\* vashrivastav AT ichf.edu.pl

Nanoelectrodes have emerged as indispensable instruments in electroanalytical chemistry, facilitating the interrogation of molecular and nanoscale phenomena that remain obscured at conventional interfaces due to ensemble-averaging effects. The diminutive dimensions of these probes grant access to accelerated mass-transport regimes, rendering them uniquely suited for resolving rapid interfacial kinetics and mapping localised electrochemical flux with unprecedented spatial resolution [1,2]. However, the high-fidelity performance of nanoprobles in Scanning Electrochemical Microscopy (SECM) is fundamentally dictated by more than mere dimensionality; the topographical smoothness and geometric fidelity of the terminal interface are paramount. Sub-nanoscale roughness and morphological irregularities can severely restrict the minimum tip-substrate separation distance, induce current instabilities, and obfuscate the quantitative deconvolution of SECM feedback. Conditionally, rigorous post-fabrication refinement is essential to ensure the reliability of the sensing interface [3].

In this work, we present a systematic framework for the architectural tailoring and in situ refinement of carbon nanoelectrodes (CNEs) optimised for nanoscale metrology. Probes featuring terminal radii between 20 and 50 nm were fabricated via the laser-assisted pulling of quartz capillaries, followed by the deposition of an electroactive carbon phase through a high-temperature acetylene pyrolysis protocol (1300-1500 °C) under a protective argon atmosphere. The structural integrity and functional viability of these nascent probes were rigorously validated using scanning electron microscopy (SEM) and cyclic voltammetry.

To circumvent the stochastic challenges associated with traditional mechanical polishing at the nanoscale, a novel SECM-guided interfacial refinement strategy was implemented. This approach utilises the high-precision positioning of the SECM to bring the CNE into controlled proximity with a rigid substrate; deliberate lateral translation was then employed to achieve a gradual, mechanically-induced metamorphosis of the electrode geometry. This refinement process was monitored via real-time electrochemical feedback, allowing for the dynamic optimisation of the electrode's active area and the realisation of a well-defined, planar nanodisk geometry.

---

**KEYWORDS:** Carbon nanoelectrodes, Scanning electrochemical microscopy, Nanoscale

---

### REFERENCES

- [1] J. Heinze, Ultramicroelectrodes in Electrochemistry. *Angew. Chem. Int. Ed. Engl.* 1993, 32 (9), 1268-1288.
- [2] J.T. Cox, B. Zhang. *Annual review of analytical chemistry* 2012, Jul 19;5(1):253-72.
- [3] P. Elsamadisi, Y. Wang, J. Velmurugan, M.V. Mirkin, *Analytical Chemistry*, 2011, 83, 671-673.

## Hall-Petch effect in the intense plastic deformation zone during FSW of magnesium alloys

M. Khokhlov<sup>1</sup>\*, J. Khokhlova<sup>1</sup>, V. Kostin<sup>1</sup>, O. Puzrin<sup>1</sup>

1) E.O. Paton Electric Welding Institute, Ukraine

\* maksymkhokhlov AT gmail.com

In previous studies, the formation of a stress-strain state during friction stir welding (FSW) of Mg alloys was modeled as a thermodynamic macro process at three linear speeds and a constant rotation rate [1, 2]. A 300% increase in the elastic modulus (E) and microhardness (H) in the stir zone was observed at the minimum linear welding speed. The elasticity values were used in the residual stresses and deformation model. The indentation data characterizes the stiffness of interatomic bonds [3], and residual stresses are the macroscopic result of plastic deformation and thermal gradients. Hence, the next study was to supplement the vision of the stress-strain state formation mechanism during FSW through visualization of the atomic structure of the Mg-Al alloy by the MD method (Chemsite 3.1.) and to study the Hall-Petch effect [4], according to which the hardness increases with a decrease in the grain size in the core zone of the FSW joint. Also, the inverse Hall-Petch effect was determined, in which the dependence of strengthening due to grain refinement is disrupted. Indentation was carried out according to ISO 14577-1:2015 with automatic determination of microhardness (H) and elastic modulus (E) by a trihedral Berkovich indenter on a computerized hardness tester.

Structural-phase components of the alloys with 92.6-95.1% Mg and 3.8-5% Al: the main solid solution  $\alpha$ -Mg matrix, hexagonal close-packed atomic lattice,  $E = 44-45$  GPa; intermetallic  $\beta$ -Mg<sub>17</sub>Al<sub>12</sub> (formed upon cooling from the liquid state in the eutectic zone), cubic atomic lattice,  $E = 65-95$  GPa [5]. During FSW five gliding modes are activated in the hexagonal crystal lattice of the  $\alpha$ -Mg matrix, which causes extreme degrees of deformation without destruction of the material shape. The denser  $\beta$ -Mg<sub>17</sub>Al<sub>12</sub> phase with cubic crystal lattice is a hard and brittle intermetallic phase, which provides strengthening in Mg-Al alloys due to plasticity (Young's modulus increases with increased pressure), i.e. resistance to volumetric and shear deformations and stiffness increase. The phase does not deform up to the brittle-plastic transition at a temperature of 300°C.

Thermodynamic processes during FSW form a typical dense junction of the mixing zone with the thermo-mechanically affected zone on the advancing side. The base alloy contains a typical rolled microstructure with coarse grains, which is preserved in the heat-affected zone. The non-uniform field of the plastic flow of metal changes the microstructure radically, so the lowest level of hardness is observed here, which makes it a critical zone for tensile failure. Local flows of a close-to-nanoscale texture (inv. Hall-Petch effect) with reduced hardness are formed at the top of the stirring zone, and at the bottom of the core (nugget zone) the crushed texture has a 300% increase in hardness. Thus, reducing the level of the stress-strain state with no Hall-Petch effects determines the most effective of the three FSW modes.

**KEYWORDS:** Hall-Petch effect, FSW, Stir zone, Hardness, Mg alloy

### REFERENCES

- [1] M.A. Khokhlov, V.A. Kostin, J.A. Khokhlova, A.G. Poklaytskiy, O.O. Makhnenko. Modeling of temperature fields distribution and stress-strain state of Mg-Al alloy FSW joints. Proceedings of the VIIth International Conference on Welding and Related Technologies (WRT 2024, 7-10 October 2024, Yaremche, Ukraine). 136-139. doi: 10.1201/9781003518518-28.
- [2] V. Kostin, J. Khokhlova, M. Khokhlov, A. Makhnenko and O. Puzrin, "Formation of Nanostructures in the Weld Nugget Zone in Friction Stir Welding of Mg-Al Alloys," 2023 IEEE 13th International Conference Nanomaterials: Applications & Properties (NAP), Bratislava, Slovakia, 2023, pp. IMT04-1-IMT04-5, doi: 10.1109/NAP59739.2023.10311017.
- [3] P. Zhang, S. Li, Z. Zhang, General relationship between strength and hardness. Materials Science and Engineering: A, 529, 62-73. <https://doi.org/10.1016/j.msea.2011.08.061> (2011).
- [4] B.R. Kuhr, K.E. Aifantis, Interpreting the inverse Hall-Petch relationship and capturing segregation hardening by measuring the grain boundary yield stress through MD indentation. Materials Science and Engineering: A, 745, 107-114. <https://doi.org/10.1016/j.msea.2018.12.053> (2019).
- [5] J. Weiler, The role of the Mg<sub>17</sub>Al<sub>12</sub>-phase in the high-pressure die-cast magnesium-aluminum alloy system. Journal of Magnesium and Alloys, 11(11), 4235-4246. <https://doi.org/10.1016/j.jma.2023.08.011> (2023).

## Stability of secondary phase in Zr-Sn alloys under irradiation: Phase-field modeling

V. Kharchenko<sup>1\*</sup>, D. Kharchenko<sup>1</sup>, A. Dvornichenko<sup>2</sup>

1) Institute of Applied Physics National Academy of Sciences of Ukraine, Ukraine

2) Sumy State University, Ukraine

\* vasilij AT ipfcentr.sumy.ua

We present a comprehensive phase-field study of microstructure evolution in Zr-Sn alloys with explicit consideration of point defects and irradiation effects. The model is formulated within a thermodynamically consistent framework based on the Gibbs free energy functional, incorporating configurational entropy, excess interaction terms, and vacancy contributions. Both equilibrium and irradiation-induced processes are analyzed, including defect production, recombination, clustering, and elastic interactions with the matrix.

At the stage of thermal treatment of solid solution the model predicts phase separation of a supersaturated solid solution with the formation of Sn-enriched precipitates of secondary phase. Numerical simulations demonstrate that these domains nucleate and grow due to diffusion-driven instabilities, followed by a coarsening regime governed by diffusion-limited kinetics. The mean particle size exhibits an algebraic growth law, and the resulting size distribution remains close to Gaussian with moderate dispersion. Equilibrium vacancies are shown to localize preferentially within domains of secondary phase, indicating strong coupling between compositional and defect fields.

It is shown that irradiation significantly modifies microstructure stability depending on the dose rate. At low dose rates, the phase structure remains largely stable, with only minor interface broadening due to ballistic mixing. Vacancies are redistributed within existing precipitates without substantial alteration of phase morphology. In contrast, at elevated dose rates, pronounced microstructural changes occur, including partial dissolution of secondary phase precipitates at early stages and subsequent reformation driven by radiation-enhanced diffusion. Nonequilibrium vacancies tend to form high-density clusters within Sn-rich regions, indicating the onset of defect aggregation and potential loop formation.

Statistical analysis based on concentration dispersions and domain size evolution reveals that irradiation induces nontrivial kinetic regimes. In particular, increased dose rates lead to a reduction in compositional fluctuations and enhanced vacancy clustering. The competition between ballistic mixing and radiation-enhanced diffusion governs the long-time behavior, resulting in stationary microstructures characterized by modified precipitate sizes and distributions.

The proposed model provides a consistent description of coupled phase transformation and defect dynamics in Zr-Sn alloys and can be used to predict microstructure stability under irradiation, which is essential for understanding the performance of nuclear fuel cladding materials.

---

**KEYWORDS:** Zr-Sn alloys, Phase-field model, Radiation-induced defects, Microstructure evolution

---

**ACKNOWLEDGEMENTS:** The work was supported by the Ministry of Education and Science of Ukraine (grant No. 0124U000551)

## Phase-field modeling of radiation effects in Nb-Sn alloys: Stability of the $A_{15}$ phase and defect-driven microstructure evolution

D. Kharchenko<sup>1\*</sup>, V. Kharchenko<sup>1</sup>, A. Dvornichenko<sup>2</sup>

1) Institute of Applied Physics National Academy of Sciences of Ukraine, Ukraine

2) Sumy State University, Ukraine

\* dikh AT ipfcentr.sumy.ua

A comprehensive phase-field model is developed to investigate microstructure evolution and radiation effects in binary Nb-Sn alloys with a focus on the formation and stability of the  $A_{15}$  ( $Nb_3Sn$ ) phase. The model is based on a thermodynamically consistent Gibbs free energy functional that incorporates chemical contributions, configurational entropy, excess interaction terms, and gradient energy effects. The system is described using coupled conserved fields corresponding to Nb and Sn concentrations, as well as vacancy concentration, allowing for a detailed representation of diffusion-driven phase transformations.

Vacancy formation, vacancy-atom interactions, and their coupling with local composition are explicitly included, enabling the transition from a binary to an effective ternary (Nb-Sn-vacancy) system. The model is further extended to describe irradiation conditions by incorporating production of nonequilibrium point defects, their recombination, annihilation at sinks, and clustering into defect loops. A reaction-rate theory framework is employed to capture the interplay between defect dynamics and microstructure evolution.

Numerical simulations are performed to study the precipitation of the  $A_{15}$  phase during thermal treatment of solid solution and its subsequent evolution under neutron irradiation. During the thermal treatment the system undergoes phase decomposition with the formation of  $A_{15}$  domains enriched in tin, exhibiting growth and coarsening behavior consistent with experimental observations. Under irradiation, a pronounced dissolution of  $A_{15}$  domains is observed at low doses, followed by defect-driven coarsening and morphological transformations at higher doses. Tin segregation and vacancy trapping lead to the formation of elongated structures and spatial redistribution of defects.

Statistical analysis reveals a decrease in niobium ordering within the  $A_{15}$  phase and enhanced tin segregation under irradiation. The evolution of vacancy concentration demonstrates preferential accumulation within  $A_{15}$  domains. The mean size of  $A_{15}$  particles significantly decreases with increasing dose, indicating radiation-induced destabilization of the ordered phase.

---

**KEYWORDS:** Phase-field modeling, Nb-Sn alloys,  $A_{15}$  phase, Radiation effects, Microstructure evolution

---

**ACKNOWLEDGEMENTS:** This work is supported by the Ministry of Education and Science of Ukraine (Project No. 0124U000551)

## Kinetics and key features of electrophysical properties in diluted aqueous colloidal solutions of $C_{60}@H_2O_n$ fullerene complexes

R. Basnukaeva<sup>1\*</sup>, A. Dolbin<sup>1</sup>, M. Vinnikov<sup>1</sup>, L. Buravtseva<sup>1</sup>, S. Cherednichenko<sup>1</sup>

*1) B. Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine, Ukraine*

\* razeta9556 AT gmail.com

Diluted aqueous colloidal solutions of  $C_{60}@H_2O_n$  prepared using the cryogenic vacuum-sublimation method were studied with respect to the kinetics of their dielectric loss tangent ( $\delta$ ) and permittivity ( $\epsilon$ ) [1]. A stock colloidal solution of hydrated fullerene  $C_{60}@H_2O_n$  containing 3 mg of  $C_{60}$  per liter was prepared by melting the solid hydrate phase produced by co-condensation of fullerene vapor and water on a liquid-nitrogen-cooled substrate. Dilute solutions of  $C_{60}@H_2O_n$  were obtained by adding a  $C_{60}@H_2O_n$  solution with a base concentration to pure distilled water and subsequent stirring with a magnetic stirrer for 1 minute. In this way, solutions with relative concentrations to the base of 1:10, 1:100, and 1:1000 were obtained. Changes in the dielectric loss tangent and permittivity over time were studied for each solution in the frequency range of 100-104 Hz. Measurements showed that the dielectric loss tangent of the colloidal  $C_{60}@H_2O_n$  solution is significantly higher than that of pure water, with its maximum shifted toward higher frequencies. This effect is presumably associated with the formation of metastable spherical hydration layers around fullerene molecules, caused by donor-acceptor interactions between  $H_2O$  molecules and the  $C_{60}$  surface [2]. The permittivity of the  $C_{60}@H_2O_n$  solution was also found to be higher than that of pure water, which is most likely due to the enhanced polarization of  $H_2O$  molecules induced by fullerene molecules. A gradual increase in both the dielectric loss tangent and permittivity was observed over time. This behavior can be attributed to the progressive formation and growth of hydration shells around  $C_{60}$  molecules. The magnitude of the observed effect depends on the concentration of fullerene in the solution and may be of interest for further biophysical investigations.

**KEYWORDS:** Hydrated fullerene  $C_{60}@H_2O_n$ , Colloidal aqueous solutions, Dielectric loss tangent, Hydration shells, Fullerene-water interactions

### REFERENCES

- [1] N.A. Vinnikov, S.V. Cherednichenko, A.V. Dolbin, V.B. Eselson, V.G. Gavrilko, R.M. Basnukaeva, A.M. Plokhhotnichenko, "The new approach for obtaining aqueous solutions of fullerene  $C_{60}@H_2O_n$  by the cryogenic sublimation method", *Low Temp. Phys.* 48, 336 (2022).
- [2] J. Herna'ndez-Rojas, J. Breto'n, and J. M. Gomez Llorente, "Global Potential Energy Minima of  $C_{60}(H_2O)_n$  Clusters", *J. Phys. Chem. B*, 110, 13357-13362 (2006).

## A robust software platform for high-resolution morphometric analysis of AFM data in nanostructured materials and nanoelectronics

A. Dvornichenko<sup>1</sup>\*, V. Kharchenko<sup>2</sup>, Y. Rozghon<sup>1</sup>

1) Sumy State University, Ukraine

2) Institute of Applied Physics National Academy of Sciences of Ukraine, Ukraine

\* a.dvornichenko AT mss.sumdu.edu.ua

An advanced software framework has been developed for automated morphometric analysis of nanostructures based on atomic force microscopy (AFM) images and deployed on the Streamlit Cloud platform. The proposed application enables a fully automated end-to-end image analysis workflow by integrating computer vision techniques, classical statistical methods, and modern machine learning approaches.

The functionality of the framework includes statistical analysis of AFM images, multilevel image segmentation for object identification across varying intensity thresholds, and comprehensive characterization of the extracted structures, including their geometric properties and spatial arrangement. In addition, clustering algorithms based on multiple morphometric descriptors have been implemented. In particular, the incorporation of the K-Means algorithm ensures efficient separation of objects in a multidimensional feature space, allowing for clear discrimination between primary nuclei and mature nanocrystallites.

The software is specifically designed for high-resolution morphometric analysis of nanostructured surfaces. It incorporates preprocessing capabilities such as image cropping to focus on regions of interest, filtering of segmented objects based on size criteria, exclusion of edge-located structures (which is critical for microscopy data), and implementation of periodic boundary conditions for the analysis of numerical simulation results describing the spatial evolution of physical systems.

The developed framework has been validated using experimental AFM images of nanostructured surfaces. The integrated analysis performed within the application demonstrates high reproducibility of topological parameters, confirming the robustness of the platform as a reliable tool for predicting the properties of advanced nanomaterials for nanoelectronic applications. The obtained results show strong agreement with experimental observations, while statistical verification confirms the adequacy of the derived distributions.

The use of a fully automated analysis pipeline significantly enhances the reliability of the results by minimizing operator-dependent bias and ensuring reproducibility.

---

**KEYWORDS:** Nanostructured thin films, Morphometric analysis, Statistics, Machine learning

---

**ACKNOWLEDGEMENTS:** This work is supported by the Ministry of Education and Science of Ukraine (Project No. 0126U000589)

## Peculiarities of the crystal structure and electron transport properties of CoFeBMoGeMn high-entropy thin-film alloy

O. Pylypenko<sup>1\*</sup>, O. Hunbin<sup>1</sup>, I. Volk<sup>1</sup>, Y. Shkurdoda<sup>1</sup>, I. Pazukha<sup>1</sup>

1) Sumy State University, Ukraine

\* o.pilipenko AT aph.sumdu.edu.ua

High-entropy alloys (HEAs) belong to a class of advanced multifunctional materials, which typically consist of five or more elements in approximately equal molar ratios (equiatomic HEAs) [1]. Non-equiatomic alloys have recently gained popularity; in these alloys, the elements are present in different molar ratios, allowing for a more flexible approach to developing alloys with unique functional characteristics that equiatomic alloys cannot achieve [2]. By varying the concentrations of individual components, it is possible to produce not only solid solutions but also intermetallics and ceramic compounds. This opens a wide range of possibilities for optimizing functional properties.

The high-entropy thin film  $\text{Co}_{10}\text{Fe}_{31}\text{B}_{10}\text{Mo}_{32}\text{Ge}_8\text{Mn}_9$  (hereafter all compositions are given in atomic percent) was deposited onto glassy carbon substrates at room temperature using a magnetron sputtering co-deposition technique from three independent sources ( $\text{Mo}_{78}\text{Ge}_{22}$ ,  $\text{Co}_{20}\text{Fe}_{60}\text{B}_{20}$ , and Mn with target purity 99.99%) in an Orion 8 system. The base pressure in the vacuum chamber was  $7 \times 10^{-8}$  Torr. During deposition, the chamber was filled with high-purity argon (99.999%, Messer) at a flow rate of  $18 \text{ cm}^3 \text{ min}^{-1}$ , maintaining a constant working pressure of 3 mTorr. The average deposition rate was approximately  $0.6 \text{ nm} \cdot \text{min}^{-1}$ . The films were annealed in an Ar+H<sub>2</sub> (2%) atmosphere using a tubular furnace under continuous gas flow. The heating rate during annealing was  $5 \text{ }^\circ\text{C min}^{-1}$ . The microstructure of the HEA films was investigated using a JEOL 2100F UHR transmission electron microscope (TEM) operated at 200 kV.

Analysis of the crystal structure of HEA films was performed after deposition and annealing at 300, 450, and 650 °C. It was demonstrated that the crystal structures of the as-deposited and annealed at 300 and 450 °C samples are amorphous. Two diffuse rings corresponding to the (111) and (200) planes of the cubic structure, with interplanar spacings  $d_{111} = 0.232 \text{ nm}$  and  $d_{200} = 0.142 \text{ nm}$ , can be identified in the diffraction patterns. These data are close to the face-centered cubic structure of Mo. After annealing at 650 °C, significant changes occur in the crystal structure of the samples. The results of the diffraction pattern analysis indicate the formation of a multi-phase composition comprising tetragonal, hexagonal, and cubic crystal structures.

The nature of the temperature dependence of the resistivity during heating confirms that defect healing and the recrystallization process occur during heat treatment. A metallic-like temperature dependence of resistivity is observed during sample cooling. Consequently, the charge-transport processes in the HEA films are driven by the scattering of conduction electrons at grain boundaries, impurities, and phonons, which is typical of electrically continuous metallic films. The high defectiveness of the sample structure results in a resistivity of about  $10^{-6} \text{ fi} \cdot \text{m}$ . The temperature coefficient of resistance is of the order of  $10^{-4} \text{ }^\circ\text{C}^{-1}$ .

---

**KEYWORDS:** High-entropy thin-film alloy, Crystal structure, Annealing, Resistivity, Temperature coefficient of resistance

---

**ACKNOWLEDGEMENTS:** This work was funded by the National Research Foundation of Ukraine under project No. 2025.07/0115.

---

### REFERENCES

- [1] M.C. Gao, D.B. Miracle, D. Maurice, X. Yan, Y. Zhang, and J.A. Hawk, “High-entropy functional materials”, *J. Mater. Res.*, 33, 3138 (2018).
- [2] X. Wang, W. Guoa and Y. Fu, “High-entropy alloys: emerging materials for advanced functional applications”, *J. Mater. Chem. A*, 9, 663 (2021).

## Morphology of island-like films obtained by electron beam evaporation

O. Pylypenko<sup>1</sup>, B. Kurylov<sup>1</sup>, I. Pazukha<sup>1</sup>, L. B. Loboda<sup>2</sup>, Y. Shkurdoda<sup>1\*</sup>

1) Sumy State University, Ukraine

2) Sumy National Agrarian University, Ukraine

\* y.shkurdoda AT aph.sumdu.edu.ua

The study of the surface morphology of island films is a highly relevant field in modern solid-state physics, materials science, and nanotechnology. This is because the physical properties of thin films in the early stages of growth differ significantly from those of continuous films and solid materials [1]. The substrate with the island film deposited on it constitutes a single, substantially heterogeneous system in many physical processes. It is necessary to take into account the properties of the film-substrate interface, as well as the properties of the substrate's surface layer. Besides, an important characteristic of films is their non-equilibrium shape and structure. Consequently, once the growth process is complete, various relaxation processes take place within the islets, the kinetics of which depend, in particular, on external influences. As a result of these irreversible changes, the film's physical properties tend towards thermodynamic equilibrium values [2].

Technologically, magnetron sputtering and electron beam sputtering are used to form nanoisland systems. The fundamental difference between these methods, which determines the properties of the resulting structures, lies in the particles' energies and the angles at which they strike the substrate. In our case, the island-like structures of ferromagnetic metals (Fe, Co, Ni) and alloys ( $\text{Fe}_x\text{Ni}_{100-x}$ ,  $\text{Co}_x\text{Fe}_{100-x}$ ) were obtained by exposing a polished glass substrate to a vapor stream of these metals for (1-10) seconds. The diffusive mobility of the atoms on the substrate was limited, as the film was deposited onto a neutral, non-oriented substrate at a temperature close to room temperature.

Based on electron microscopy results, it can be concluded that during film deposition, a large number of fine crystallization nuclei form and grow simultaneously. As a result, the unburned films, regardless of their composition and thickness, exhibited virtually identical structures. The islands are irregularly shaped and measure 2-5 nm, whilst the gaps between them appear as channels of roughly the same width, 1-2 nm. Thus, the Folmer-Weber growth mechanism is at work in the films. Structurally, the increase in the effective thickness of the films manifests itself solely in an increase in the density of the islands.

Significant morphological changes in the nanoisland systems occur following annealing at 700 K and are determined by their effective thickness. At a small effective thickness of 3-5 nm, the only change observed is an increase in the size of the islands to 10-20 nm due to coalescence. At the same time, the total number of islets is reduced by a factor of 3-5, leading to an increase in channel width to 2-7 nm. At an effective thickness of 6-7 nm, a similar pattern is observed, with a higher island density and narrower channels of 2-5 nm. Subsequently, as the effective thickness increases to 8-10 nm, a 'bridge-like' structure forms in both pure metal films and alloy films.

---

**KEYWORDS:** Island films, Morphology, Magnetic materials, Electron-beam evaporation

---

**ACKNOWLEDGEMENTS:** This work was funded by the State Program of the Ministry of Education and Science of Ukraine (Project No. 0125U001561).

---

### REFERENCES

- [1] S. Chen, D. Rong, Ya. Shang, M. Cai, X. Li, Q. Zhang, S. Xu, Y. Xu, H. Gao, H. Hong, T. Cui, Q. Jin, J. Wang, L. Gu, Q. Zheng, C. Wang, J. Zhang, G. Liu, K. Jin, and E. Guo, "Magnetic Nanoislands in a Morphotropic Cobaltite Matrix", *Adv. Func. Mater.*, 33, 2302936 (2023).
- [2] M. Saccone, J. C. Gartside, K. D. Stenning, W. R. Branford, and F. Caravelli, "From Vertices to Vortices in magnetic nanoislands", *Phys. Fluids*, 35, 017101 (2023).

## Nanotextured ammonium dihydrogen phosphate for NLO applications

A. Bendak<sup>1</sup>, J. Lang<sup>2</sup>, S. Taboukhat<sup>2</sup>, I. Teslyuk<sup>3</sup>, V. Adamiv<sup>3</sup>, D. Guichaoua<sup>2</sup>, A. Andrushchak<sup>1\*</sup>, B. Sahraoui<sup>2</sup>

1) Lviv Polytechnic National University, Ukraine

2) University of Angers, France

3) Ivan Franko National University of Lviv, Ukraine

\* anatolii.s.andrushchak AT lpnu.ua

The design of novel materials is significant and intriguing task. One of the possible approaches for new structures creating is composition of two or several materials in specific way. Such a task can be resolved by providing of guest material into host matrix. The concept of the present research is creation of nanostructured material that is porous template filled with crystallites. To prepare the defined composition, nanoporous anodic alumina oxide (AAO) membranes and ammonium dihydrogen phosphate (ADP) compounds were used. Somewhat similar investigations are presented in works [1, 2]. In this research we examined new techniques of sample preparation, that leads to exceptional structural and functional characteristics of obtained materials. The synthesis process of nanostructures based on AAO template filled with ADP as well as structural and non-linear optical (NLO) properties of synthesized material was studied. The formation of crystalline nanoarchitectures was established via scanning electron microscopy and X-ray diffraction methods. The performed research on the synthesized samples shows the formation of ADP nanoarchitectures which exhibits structural sustainability and NLO efficiency. Therefore, the integration process of functional material with nanoporous membrane represent a method for creation of nanotextured composition with origin physical properties.

---

**KEYWORDS:** Ammonium dihydrogen phosphate (ADP), Nonlinear optics, Anodic alumina templates, Nanocomposites

---

**ACKNOWLEDGEMENTS:** The presented results are part of the TeraHertz project that has received funding from the HORIZON-MSCA-2021-SE-01 Program, agreement number 101086493.

---

### REFERENCES

- [1] N. Andrushchak, V. Adamiv, V. Haiduchok, I. Teslyuk, Y. Yashchyshyn and A. Andrushchak, "Transmission Spectra Investigation of Nanoporous Al<sub>2</sub>O<sub>3</sub> Matrices Filled with KDP, ADP and TGS Crystals at Visible, NIR, and SubTerahertz Ranges," 2021 IEEE 11th International Conference Nanomaterials: Applications & Properties (NAP), pp. 1-5, 2021.
- [2] D. Guichaoua, W. Alnusirat, V. Adamiv, N. Andrushchak, I. Teslyuk, D. Shulha, A. Andrushchak, I. Gnilitskyi and B. Sahraoui, "Nonlinear optical properties of some nanosized ammonium dihydrogen phosphate crystals incorporated in aluminum oxide nanopores", AIP Advances 14 (11): 115314, November 2024.

## Thermal stability and microstructural evolution of transition-metal-alloyed Al-Mg alloys produced by melt spinning

T. Monastyrska<sup>1\*</sup>, A. Berezina<sup>1</sup>, O. Molebnyi<sup>1</sup>, A. Kotko<sup>2</sup>

1) G.V. Kurdyumov Institute for Metal Physics of the NAS of Ukraine, Ukraine

2) Frantsevich Institute for Problems of Materials Science of the NAS of Ukraine, Ukraine

\* monast AT imp.kiev.ua

The decomposition of supersaturated solid solutions of Al-Mg alloys containing transition metals has been studied in this work. Al-Mg alloys, additionally alloyed with Sc, Zr, Hf, and Cr, were obtained by the melt-spinning method in the form of rapidly quenched ribbons at the quenching temperature of 1000 °C. The annealing at the temperature range of 300-450 °C was carried out to study aging processes in the alloys. The structure and mechanical properties of the alloys were studied using transmission electron microscopy, X-ray diffractometry, and hardness measurements. The temperature intervals of the phase transformations were determined by measuring the temperature coefficient of resistivity,  $\alpha_t = 1/\rho_0 \cdot d\rho/dT$ . For rapidly quenched ribbons of Al-Mg-Sc-Zr-Hf-Cr alloys, the change in the temperature coefficient of electrical resistance  $\alpha_t = 1/\rho_0 \cdot d\rho/dT$  was investigated during continuous heating at the rate of 3°/min in the range from room temperature to 550 °C.

The decomposition of supersaturated solid solutions is continuous, with the precipitation of nano-sized spherical Al<sub>3</sub>X (X - Sc, Zr, Hf) particles of 10-50 nm. Two-stage heat treatment of ribbons, which underwent 300 °C × 10 hours + 400 °C × 10 hours heat treatment, makes it possible to increase the hardness of Al-Mg-Sc-Zr-Hf-Cr alloys up to 50% in comparison with isothermal aging at 400 °C for 10 hours. Additional alloying with Cr not only increases the strength properties of the alloys but also increases their thermal stability. The temperature range of phase transformations at alloying by Hf does not shift, but mainly widens to higher temperatures, and Cr effect results in a shift of almost 70 °C toward higher temperatures.

---

**KEYWORDS:** Al-Mg alloys, Melt spinning, Anomalously supersaturated solid solution, Precipitation strengthening

---

**ACKNOWLEDGEMENTS:** This work was carried out within the framework of budget project 056/21 of the G.V. Kurdyumov IMP of the N.A.S. of Ukraine

## Influence of magnetic field post-treatment on electrical properties of polymer composites with hybrid filler

O. Maruzhenko<sup>1\*</sup>, Y. Mamunya<sup>2</sup>, I. Paraschenko<sup>2</sup>, A. Misiura<sup>1</sup>, D. Sokoliuk<sup>1</sup>, K. Olszowska<sup>3</sup>, U. Szeluga<sup>3</sup>

1) E.O. Paton Electric Welding Institute of the National Academy of Sciences of Ukraine, Ukraine

2) Institute of Macromolecular Chemistry of the National Academy of Sciences of Ukraine, Ukraine

3) Center of Polymer and Carbon Materials, Polish Academy of Sciences, Poland

\* a.v.maruzhenko AT gmail.com

The wide range of properties exhibited by polymer composites makes them suitable for use in a variety of applications. Thermoplastic-based composites can be processed and treated after formation. Thus, the formed composite structure can be modified by remelting the material and creating a new structure in the melted state. The aim of this work was to investigate the effect of random and segregated distribution, followed by treatment of the samples in a magnetic field, on the electrical properties of polymer composites. For the study, an LDPE thermoplastic polymer matrix and two types of filler were selected: dispersed nickel (2 vol. %) and a hybrid nickel/anthracite mixture (1/1 vol. %). The statistical 3D distribution was obtained using a disc-type micro-extruder, and the segregated 3D structure was obtained by mixing the polymer and filler powders with the following hot compaction. The one-dimensional 1D structure was obtained by treatment of the composites with the 3D statistical and segregated distribution in a magnetic field at 140 °C in the melted state. The magnetic induction at the sample location was 0.5 T. The DC electrical conductivity of the composites was determined using an E<sub>6</sub>-13A teraohmmeter, and the dielectric constant, was measured at a frequency of 1 kHz using an E<sub>8</sub>-4 digital capacitance meter. Optical microscopy revealed that the samples' treatment in a magnetic field significantly affected their morphology. The ferromagnetic Ni filler aligned itself within the polymer melt along the magnetic field lines. This significantly impacted the electrical properties of the composites, with the dielectric constant's dependence on electrical conductivity being empirically established and analytically described. The influence of the samples' treatment in a magnetic field on these parameters was also demonstrated, particularly the dielectric-conductor transition was observed in a composite with a 1D structure based on a 3D segregated composite containing 2 vol.% of Ni. Composites with hybrid filler demonstrate a stronger dependence of the dielectric constant on the electrical conductivity.

**KEYWORDS:** Polymer composites, Hybrid fillers, Electrical conductivity, Magnetic-field alignment, Segregated structure

## Delineate the role of interaction in biosensing: Size-tuned metal nanoparticles controlling enzyme activity for smart biosensors

P. Bhardwaj<sup>1</sup> \*

1) *AcSIR, CSIR-IMTECH, Chandigarh, India, India*

\* priyabhardwajpb1993 AT gmail.com

The nanomaterial-based biosensors require a precise understanding of nano-bio interactions, particularly the influence of nanoparticle size on enzyme structure and function. In this work, we report a comprehensive investigation of size-dependent interactions between silver nanoparticles (AgNPs; 5-100 nm) and urease, a model metalloenzyme, employing spectroscopic, thermodynamic, and activity-based analyses. Interaction studies revealed a strong dependence of binding affinity and inhibition mechanism on nanoparticle size. Small AgNPs (5 nm) exhibited the highest binding affinity ( $K_d \sim 66$  nM), inducing significant conformational alteration in urease, as confirmed by circular dichroism. In contrast, intermediate sizes (20 and 50 nm) showed weaker binding ( $K_d \sim 712$  and  $616$  nM) and minimal structural perturbation. Notably, larger AgNPs (100 nm) demonstrated strong binding ( $K_d \sim 171$  nM) without significant conformational change, suggesting inhibition via surface adsorption and active-site masking. Thermodynamic profiling using isothermal titration calorimetry highlighted distinct interaction modes: exothermic binding for 5 and 100 nm particles, and endothermic signatures for mid-sized nanoparticles, attributed to hydration layer formation at the nano-bio interface. The enzyme inhibition assays demonstrated that both smallest and largest nanoparticles achieve maximum inhibition at low concentrations, albeit through distinct mechanisms- structural denaturation and steric blocking, however, intermediate sizes are less effective. This study establishes nanoparticle size as a critical design parameter governing enzyme interaction pathways, binding thermodynamics, and functional inhibition. The findings provide a framework for engineering nanomaterial-enabled biosensors and therapeutic inhibitors with tunable activity, highlighting the importance of size-controlled nanostructures in advanced biomedical and environmental applications.

---

**KEYWORDS:** Silver nanoparticle, Urease, Nano-Bio interaction, Enzyme inhibition

---

**ACKNOWLEDGEMENTS:** The author thanks UGC fellowship for providing funds.

---

### REFERENCES

- [1] M. Choudhary, B. Bisht, J. K. Saini, Bharti, P. Singh, P. Bhardwaj, R. Dilawari, A. K. Pinnaka, P. Ray, M. Gupta, S. Sethi, C. R. Suri, M. Raje and V. Bhalla, “Bifunctionalized nanobioprobe based rapid color-shift assay for typhoid targeting Vi capsular polysaccharide”, *Biosensor and Bioelectronics*, 228, 115195 (2023).
- [2] P. Bhardwaj, B. Bisht, V. Bhalla “Nanoscale size impact of nanoparticle interaction and activity studies with urease”, *Nanoscale*, 17(9), 5000-5004 (2025).
- [3] S. Tadepalli, Z. Wang, J. Slocik, R. R. Naik and S. Singamaneni, “Effect of size and curvature on the enzyme activity of bionanoconjugates” *Nanoscale*, 2017, 9, 15666-15672 (2017).

## Direct synthesis of graphene on dielectric substrates using plasma enhanced chemical vapor deposition

M. A. Saeed<sup>1\*</sup>, M. A. Saeed<sup>1\*</sup>

*1) Institute of Materials Science, Kaunas University of Technology, Lithuania*

\* muhammad.saeed AT ktu.lt

The development of high-performance biosensors is essential for advancing medical diagnostics, environmental monitoring, and point-of-care testing. Graphene has emerged as a promising biosensing material due to its exceptional electrical, mechanical, and biocompatible properties. However, conventional graphene synthesis methods often require complex transfer processes that introduce defects and contamination, limiting device performance. This study investigates the direct growth of graphene using Plasma-Enhanced Chemical Vapor Deposition (PECVD), eliminating the need for transfer and preserving graphene's intrinsic properties. PECVD enables low-temperature, catalyst-free synthesis directly on dielectric and polymer substrates, making it highly suitable for flexible and wearable biosensing applications. High-quality monolayer and few-layer graphene films were synthesized on annealed and non-annealed SiO<sub>2</sub> substrates (100 nm and 300 nm) by optimizing plasma power, precursor flow rates, and substrate temperature. Raman spectroscopy, SEM, and electrical measurements confirmed the structural quality and conductivity of the graphene films. The directly grown PECVD graphene platform demonstrates strong potential for next-generation biosensors, enabling stable, real-time, and label-free detection for advanced point-of-care diagnostic applications.

---

**KEYWORDS:** Graphene, PECVD, FETs

---

**ACKNOWLEDGEMENTS:** This research has received funding from the European Regional Development Fund under a grant agreement with the Research Council of Lithuania (LMTLT). I A. Guobienė, K. Šlapikas, M. Andrulevičius, T. Tamulevičius, gratefully acknowledges the Center of Spectroscopic Characterization of Materials and Electronic/Molecular Processes (SPECTROVERSUM Infrastructure) for the use of Raman spectrometer. Thanks to my supervisor Šarūnas Meškiniš for guiding in this work and Institute of materials science of Kaunas University of technology for providing all research facilities.

---

### REFERENCES

- [1] Meškiniš, Š., A. Vasiliauskas, A. Guobienė, M. Talaikis, G. Niaura, & Gudaitis, R. (2022). The direct growth of planar and vertical graphene on Si (100) via microwave plasma chemical vapor deposition: synthesis conditions effects. *RSC advances*, 12(29), 18759-18772.
- [2] R. Gudaitis, A. Lazauskas, Jankauskas, Š., & Meškiniš, Š. (2020). Catalyst-less and transfer-less synthesis of graphene on Si (100) using direct microwave plasma enhanced chemical vapor deposition and protective enclosures. *Materials*, 13(24), 5630.
- [3] Y.S. Kim, K. Joo, S.K. Jerng, J.H. Lee, E. Yoon, S.H. Chun, Direct growth of patterned graphene on SiO<sub>2</sub> substrates without the use of catalysts or lithography. *Nanoscale*, 6(17), 10100-10105 (2014).
- [4] Meškiniš, Š., R. Gudaitis, A. Vasiliauskas, A. Guobienė, Jankauskas, Š., V. Stankevič, ... & Žurauskienė, N. (2023). Biosensor based on graphene directly grown by MW-PECVD for detection of COVID-19 spike (S) protein and its entry receptor ACE2. *Nanomaterials*, 13(16), 2373.

## Electrospun PCL scaffolds as local amikacin delivery systems: From quantitative incorporation analysis to verification of antimicrobial activity

S. Dmytruk<sup>1\*</sup>, Y. Husak<sup>1</sup>, S. Bajkacz<sup>2</sup>, V. Kulibaba<sup>1</sup>, I. Yanko<sup>1</sup>, I. Bulyha<sup>3</sup>, F. Wojtas<sup>2</sup>, S. Kyrylenko<sup>1</sup>, V. Korniienko<sup>4,5</sup>

1) Biomedical Research Center, Academic and Research Medical Institute, Sumy State University, Sumy, Ukraine

2) Silesian University of Technology, Faculty of Chemistry, Poland

3) Sumy State University, Ukraine

4) University of Latvia, Riga, Latvia

5) Biomedical Research Center, Medical Institute, Sumy State University, Sumy, Ukraine

\* s.dmytruk AT med.sumdu.edu.ua

Electrospun nanofibrous scaffolds represent one of the most promising platforms for local drug delivery purpose due to their high porosity and morphological similarity to the extracellular matrix [1, 2]. Polycaprolactone (PCL), as a biopolymer with well-modified mechanical properties and a predictable degradation rate, shows great potential for use as such a matrix [3]. The use of electrospun PCL matrices for amikacin incorporation is considered a strategy to overcome limitations associated with drug's high hydrophilicity and short half-life. This enables the transformation of short-term antibacterial action into a prolonged therapeutic effect [4, 5].

In this study, we performed a quantitative assessment of amikacin incorporation into electrospun PCL scaffolds and verified their antimicrobial potential.

PCL scaffolds were synthesized via electrospinning at voltage of 18000 V using a rotary collector at distance of 13 cm, rotation speed of 600 rpm and solution flow rate 2 ml/h. Lyophilized amikacin was introduced directly into the electrospinning solution. A 3:1 mixture of chloroform and dimethylformamide was used to dissolve the PCL. Quantitative determination of amikacin loaded into the membrane was carried out using liquid chromatography coupled with tandem mass spectrometry (LC-MS/MS). To evaluate antimicrobial activity using the disk-diffusion method, the PCL scaffolds were punched into  $\varnothing$  6 mm discs. Growth inhibition zones were quantified for reference strains of *S. aureus*, *E. coli*, and *P. aeruginosa*.

The mean of amikacin drug loading, calculated based on chromatographic analysis data, was  $4,10 \pm 0,71\%$ , with Encapsulation Efficiency of  $79,8 \pm 13,7\%$ . These values confirm the successful retention of amikacin within the polymer matrix, which is critical for overcoming its pharmacological limitations, such as extreme hydrophilicity and a short half-life.

Amikacin-loaded PCL scaffolds demonstrated pronounced antimicrobial activity against *S. aureus*, *E. coli*, and *P. aeruginosa*. The formation of large inhibition zones (exceeding 20 mm) around scaffold discs confirms sufficient diffusion of amikacin from hydrophobic PCL matrix into the aqueous environment of agar. The slightly smaller growth inhibition zones around PCL-amikacin scaffolds compared to standard paper amikacin disks can be considered indirect evidence of a controlled delivery system in operation, where the PCL scaffold acts as a depot, limiting diffusion rate and ensuring a gradual, metered release of antibiotic throughout the incubation period. PCL scaffold creates a reliable amikacin depot potentially capable of maintaining concentrations above the minimum inhibitory level directly at the infection site for at least several days, what is significantly reduces the risk of systemic toxicity typical for aminoglycosides, and is an effective solution for enhancing wound treatment efficacy and patient safety.

**KEYWORDS:** Electrospun PCL scaffolds, Amikacin, Antimicrobial activity

**ACKNOWLEDGEMENTS:** Supported by the Ministry of Education and Science of Ukraine (Projects No. 0126U000870, 0124U000637, 0124U000552)

### REFERENCES

- [1] M. B. Reyhanoglu, R. B. Sulutas, B. Adali, E. Kaya, G. B. Tinaz, S. Evran, O. Gunduz, S. Cesur, “Electrospun Poly(lactic acid) (PLA)/ Polycaprolactone (PCL) Nanofibrous Wound Dressings Incorporating Caffeic Acid and Gentamicin for Antibacterial and Antibiofilm Applications”, *Eur. J. Pharm. Biopharm.*, vol. 223, Art. no. 115054, 2026, doi: 10.1016/j.ejpb.2026.115054.
- [2] P. Zhao, W. Chen, Z. Feng, Y. Liu, P. Liu, Y. Xie, D. G. Yu, “Electrospun Nanofibers for Periodontal Treatment: A Recent Progress”, *Int. J. Nanomedicine*, vol. 17, pp. 4137-4162, 2022, doi: 10.2147/IJN.S370340.
- [3] C. Meng, “Electrospinning PLLA/PCL Blend Fibre-Based Materials and Their Biomedical Application: A Mini Review”, *Polymers*, vol. 17, no. 20, Art. no. 2802, Oct. 2025, doi: 10.3390/polym17202802.
- [4] M. Glinka, K. Filatova, J. Kucińska-Lipka, E. D. Bergerova, A. Wasik, and V. Sedlářik, “Encapsulation of Amikacin into Microparticles Based on Low-Molecular-Weight Poly(lactic acid) and Poly(lactic acid-co-polyethylene glycol)”, *Mol. Pharm.*, vol. 18, no. 8, pp. 2986-2996, Aug. 2021, doi: 10.1021/acs.molpharmaceut.1c00193.
- [5] A. L. Alfalujji, Q. S. Kadhim, and A. A. Mahdi, “Electrospun poly( $\epsilon$ -caprolactone)/silver nanoparticle nanofibrous scaffolds with antibacterial activity for wound-dressing applications”, *RSC Adv.*, vol. 15, no. 45, pp. 37899-37907, Oct. 2025, doi: 10.1039/d5ra06746d.

## Catalytic decomposition of ammonia over graphene-based nanocomposites for green hydrogen production

A. Marinoiu<sup>1</sup>\*

1) Institute for Cryogenics and Isotopic Technologies - ICSI, Ramnicu Valcea, Romania, Romania

\* adriana.marinoiu AT icsi.ro

The transition to a carbon-neutral economy requires the synthesis and development of improved and efficient hydrogen storage and transport vectors. Ammonia has recently become a potential candidate due to its high hydrogen density and carbon-free composition. However, the well-known kinetics of ammonia decomposition are often limited by the high temperatures required as well as the high cost of the noble catalysts often used in the process.

This study explores the design of novel graphene-based nanomaterials as high-surface area supports for transition metal nanoparticles commonly used in ammonia catalysis (e.g., Ni, Co). These considerations, together with the good electronic conductivity and chemical stability of graphene oxide, demonstrate a significant improvement in the catalytic activity of Ni and Co supported on reduced graphene oxide for hydrogen production.

This study discusses the synergistic effects based on the interaction between the graphene network and metal nanoparticles, as the latter promote electron transfer, reducing the activation energy for N-H bond cleavage [1].

Regarding structural optimization, through the doping process and, we obtained a superior metal dispersion and superior thermal stability, preventing sintering of metal nanoparticles at operating temperatures specific for ammonia decomposition (450-700°C) [2], by considering a green chemistry method for synthesis.

This research highlights the potential of graphene-based engineered catalysts to provide a cost-effective and scalable solution for CO<sub>x</sub>-free hydrogen generation, indicating and positioning graphene materials close to the forefront of the hydrogen economy infrastructure in Europe.

---

**KEYWORDS:** Graphene, Ammonia decomposition, CO<sub>x</sub>-free hydrogen, Heterogeneous catalysis

---

**ACKNOWLEDGEMENTS:** This work was supported by the project PN 23 15 01 03, Contract No. 20N/2023, Core Program within the National Research Development and Innovation Plan 2022-2027, financed by Ministry of Research, Innovation, Digitization of Romania and by the project RO-HydroHub “Romanian Hydrogen and New Energy Technologies Hub”, contract nr. G2025-113330/ 2025, SMIS code: 351358, financed from European funds via the POCIDIF 2021-2027 Program, activity “A3.2 Green technology for bidirectional hydrogen-ammonia conversion”.

---

### REFERENCES

- [1] V.B. Parambath, R. Nagar, S. Ramaprabhu, Effect of nitrogen doping on hydrogen storage capacity of palladium decorated graphene. *Langmuir* 2012, 28, 7826-7833
- [2] R. Lan, J.T.S. Irvine, S. Tao, Ammonia and related chemicals as potential indirect hydrogen materials. *Int. J. Hydrog. Energy* 2012, 37, 1482-1494

## Effect of ball-milling time on In-situ formation of reinforce boride phases in AlCrTiNbVB high-entropy alloys during electron-beam sintering

S. Nakonechnyi<sup>1</sup>\*, A. Yurkova<sup>1</sup>, P. Loboda<sup>1</sup>

1) National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", Ukraine

\* nakonechny.serhiy AT edu.kpi.ua

Composite materials based on high-entropy alloys (HEAs) with in-situ inclusions of refractory compounds exhibit excellent mechanical properties, wear resistance, corrosion resistance, and other desirable characteristics [1, 2]. At the same time, a key challenge in developing such composites is the processing technology, particularly the preparation of feedstock materials (powder mixtures, compacts) and the high-temperature in-situ reactions between metallic components (Cr, Ti, Nb, V, etc.) and nonmetallic elements (B, Si, C) [3].

This study investigates the effect of mechanical alloying (MA) time on the in-situ phase formation, structure and hardness of AlCrTiNbVB HEAs consolidated by high-speed electron-beam sintering (EBS). AlCrTiNbVB HEAs were produced by MA of elemental powders using a Retsch PM<sub>100</sub> planetary mill for 1, 2, 10, and 20 hours at 400 rpm in the petrol medium. The as-prepared powders were consolidated by EBS using ELA-6 equipment under identical conditions.

After 1, 2, and 10 h of MA, the powder consists of two solid solutions (Nb- and Cr-rich) and an Al<sub>8</sub>V<sub>5</sub> intermetallic phase. After 20 h of MA, the structure evolves into two solid solutions enriched in Cr/Nb and Al/V, respectively. The Cr/Nb-enriched solid solution exhibits a nanostructured state, as evidenced by an average crystallite size of ~15 nm determined by XRD analysis. This behavior is characteristic of nanostructure formation in HEAs during MA [4, 5]. A noticeable fraction of ultrafine WC particles, obtained from the milling media, is also detected and confirmed by XRD and SEM analysis.

After EBS, the alloys exhibit a composite structure consisting of a solid solution matrix and fine boride particles. This structure results from component interactions, in-situ reactions, and the extremely high-speed sintering process (up to 3 min, including heating and cooling). At the same time, the chemical composition, size, and morphology of boride particles strongly depend on the MA time. After 1-10 h of MA and subsequent consolidation, elongated, needle-like Ti/Nb-based boride particles are formed in-situ in AlCrTiNbVB HEA. With the increase in MA time, particle fragmentation begins, leading to the formation of small, irregularly shaped particles. In comparison, after 20 h of MA and subsequent consolidation, the in-situ formation of ultrafine, cube-shaped high-entropy boride particles is observed, as confirmed by SEM and EDS analysis.

The structure evolution is directly associated with the formation of a nanostructured solid solution matrix during MA and EBS, combined with the sluggish diffusion effect of HEAs. In addition, the increasing fraction of finely dispersed boride particles and their progressive morphological and chemical changes contributes significantly to dispersion strengthening. As a result, the average hardness of the AlCrTiNbVB HEA increases from 7.36 to 12.29 GPa for powders milled for 1 and 20 h, respectively.

**KEYWORDS:** High entropy alloys, In-situ formation, Composite, Boride inclusions

**ACKNOWLEDGEMENTS:** This research was supported by the project of the Ministry of Education and Science of Ukraine, state registration number 0124U000913.

### REFERENCES

- [1] J. Guo, W. Xie, and J. Pu, "Tribocorrosion behaviors and mechanisms of in-situ TiC/TiB/Cr<sub>2</sub>B reinforced CrMnFeCoNi high-entropy alloy composite coatings prepared by laser cladding," *Ceram. Int.*, 51 (18), 26742-26756 (2025).
- [2] J. Zhang, L. Zhang, and H. Ma, "In-situ development of Ti(C, N) and their effect on microstructure, wear and corrosion properties of CoCrFeNiTi high-entropy alloy matrix composites," *Vacuum*, 221, 112914 (2024).
- [3] Z. Yu, W. Xing, C. Liu, K. Yang, H. Shao, and H. Zhao, "Construction of multiscale secondary phase in Al<sub>0.25</sub>FeCoNiV high-entropy alloy and in-situ EBSD investigation," *J. Mater. Res. Technol.*, 30, 7607-7620 (2024).
- [4] A. I. Yurkova, S. O. Nakonechnyi, V. V. Cherniavsky, and V. V. Kushnir, "Nanostructured AlCoFeCrVNi and AlCoFeCrVTi high-entropy alloys resulted from mechanical alloying and sintering," *Appl. Nanosci.*, 12 (4), 849-860 (2021).
- [5] M. Vaidya, G. M. Muralikrishna, and B. S. Murty, "High-entropy alloys by mechanical alloying: A review," *J. Mater. Res.*, 34 (5), 664-686 (2019).

## Fabrication and experimental characterizations of an SU-8 composite enhanced with silver Micro/Nano-inclusions

R. C. Voicu<sup>1</sup>\*, R. Muller<sup>1</sup>, C. Parvulescu<sup>1</sup>, R. Gavrilă<sup>1</sup>, O. Brincoveanu<sup>1</sup>

1) IMT Bucharest, Romania

\* rodica.voicu AT imt.ro

In recent years, various nano-inclusions, including metallic NP, organoclays, carbon nanotubes (CNTs), and graphene, have attracted considerable research interest for nanocomposite development. Owing to their enhanced physicochemical and functional properties, these materials have found applications across many fields, including microelectromechanical systems (MEMS), electronics [1-2], medicine, aerospace, automotive engineering, and packaging technologies [3-4].

In this paper, we present the fabrication of a nanocomposite material based on SU-8 polymer matrix reinforced with Ag micro/nano-scale inclusions. The polymeric matrix employed in this study is the epoxy-based photoresist SU-8. This material was selected due to its excellent photopatternable properties, which make it highly suitable for the fabrication of MEMS and related microscale devices. First, the Ag particles were characterized using scanning electron microscopy-SEM. The particle diameter ranged from 300 nm to 3-5  $\mu\text{m}$ , with an average particle size of about 900 nm. Subsequently, SU-8 2050 was selected as the polymeric matrix due to its high viscosity and its capability to produce layers with a wide range of thicknesses.

The nanocomposite material was prepared through the physical blending of functionalized silver particles dispersed in a wet solution with the SU-8 polymer matrix. In order to achieve a homogeneous dispersion of the metallic inclusions, the composite mixture was subjected to ultrasonic treatment, with the sonication time optimized accordingly. Additionally, manual homogenization was performed to further improve particle distribution within the matrix. The obtained nanocomposite was spin-coated onto a silicon wafer to obtain a layer with a thickness of approximately 20  $\mu\text{m}$ . Furthermore, several thermal treatment processes were carried out, following the hard baking thermal treatments at 95 °C and 185 °C used for SU-8 photoresists. Hard baking is used to enhance the stability and durability of patterned resist structures during subsequent processing steps. Optical and SEM characterizations were performed to evaluate the homogeneity and morphological properties of the fabricated composites. Energy Dispersive X-ray Spectroscopy (EDS/EDX) analyses were carried out for the compositional characterization of the material. Experimental measurements of the elastic modulus of the nanocomposites were conducted following the thermal treatments applied to the fabricated nanocomposites. An increase in the elastic modulus was observed with increasing hard-bake temperature. The obtained measurements results were subsequently compared with those corresponding to the pristine SU-8 polymer in order to assess the influence of the Ag micro/nano-inclusions and thermal treatments on the mechanical properties of the materials.

Due to their improved mechanical properties, the developed nanocomposites show significant potential for advanced applications, as for nanosensors and MEMS/NEMS.

---

**KEYWORDS:** Nanocomposite, Silver, Metals, Mechanical properties

---

**ACKNOWLEDGEMENTS:** This research was funded from the National Core Programme, Contract No 8N/2023, financed by the Romanian Ministry of Research, Innovation and Digitalization and the project "National Platform for Semiconductor Technologies", contract no. G 2024-85828/390008/27.11.2024, SMIS code 351364, co-funded by the European Regional Development Fund under the Program for Intelligent Growth, Digitization, and Financial Instruments.

---

### REFERENCES

- [1] H. Han, V. Martinez, C. Forró, J. Polesel-Maris, J. Vörös, T. Zambelli, Integration of silver nanowires into SU-8 hollow cantilevers for piezoresistive-based sensing, *Sensors and Actuators A: Physical* 301, 111748 (2020)
- [2] C. D. Gerardo, E. Cretu and R.Rohling, Fabrication of Circuits on Flexible Substrates Using Conductive SU-8 for Sensing Applications, *Sensors* 17, 1420 (2017)
- [3] R.H. Alasfar, S. Ahzi, N. Barth; V. Kochkodan; M. Khraishseh; Koç, M. A Review on the Modeling of the Elastic Modulus and Yield Stress of Polymers and Polymer Nanocomposites: Effect of Temperature, Loading Rate and Porosity. *Polymers* 14, 360, (2022)
- [4] V. Seenaa, K. Hari, S. Prajakta, R. Pratap and V. Ramgopal Rao, A novel piezoresistive polymer nanocomposite MEMS accelerometer, *J. Micromech. Microeng.* 27 015014 (2017)

## FTIR-DFT approach at the synthesis of silver-containing chalcogenide nanoparticles

A. Nikolaienko<sup>1\*</sup>, A. Dmytruk<sup>1</sup>, A. Karlash<sup>2</sup>

1) Institute of Physics, NAS of Ukraine, Ukraine

2) Taras Shevchenko National University of Kyiv, Ukraine

\* asya.nikolaenko AT gmail.com

The coordination of metal ions with ligands plays a key role in the wet chemical synthesis of semiconductor nanoparticles (NP) but remains poorly understood at the molecular level. In particular, the mechanisms of interaction between silver ions and amino acids as biologically relevant and environmentally safe ligands, such as N-acetylcysteine (NAC), require detailed spectroscopic and theoretical investigation. We address the problem of determining the preferred coordination mode of  $\text{Ag}^+$  with NAC in aqueous media.

Using a combination of Fourier transform infrared (FTIR) spectroscopy and density functional theory (DFT) calculations, we found that silver ions are predominantly coordinated simultaneously with the thiol sulfur atoms and the carbonyl oxygen atoms of NAC, although most studies report coordination of the ion with the sulfur atom only [1, 2]. Comparison of experimental and calculated IR spectra shows that this coordination mode reproduces key spectral features at the characteristic frequencies. Importantly, experimental observations show that the formation of nanoparticles occurs under both acidic ( $\text{pH} \approx 3$ ) and neutral ( $\text{pH} \approx 7$ ) conditions. Accordingly, the DFT results indicate that the preferred coordination mode of  $\text{Ag}^+$  with NAC remains unchanged in these environments. Furthermore, the results demonstrate that  $\text{Ag}^+$  coordination can induce intramolecular proton transfer from the thiol to the carboxyl group.

These data contribute to a deeper understanding of metal-ligand interactions in amino acid systems and are relevant for controlling the stages of the synthesis of silver-containing chalcogenide nanoparticles. In a broader sense, the combined FTIR-DFT approach provides a robust framework for studying coordination mechanisms in complex molecular systems and reveals nanoparticle nucleation processes.

---

**KEYWORDS:** FTIR, DFT, Metal-ligand coordination, Wet chemical synthesis, Semiconductor nanoparticles

---

**ACKNOWLEDGEMENTS:** The authors would like to thank Dr. Olena Hnatyuk for her assistance in performing IR measurements and critical discussion of the results, the Department of Physics of Biological Systems for providing access to the equipment, and Bruker Corporation for providing the spectrometer as humanitarian aid. AN and AD would like to thank the Ministry of Education and Science of Ukraine for supporting by "PhD-research project".

---

### REFERENCES

- [1] C. Abbehausen, A. Tassiele, Heinrich, Emiliana P. Abrão, Claudio M. Costa-Neto, Wilton R. Lustri, André L.B. Formiga, Pedro P. Corbi, Chemical, spectroscopic characterization, DFT studies and initial pharmacological assays of a silver(I) complex with N-acetyl-L-cysteine, *Polyhedron*, 30, 579-583 (2011)
- [2] S. P. Santos, I. K. Chandra, F. E. Soetaredjo, A. E. Angkawijaya, and Yi-Hsu Ju, Equilibrium Studies of Complexes between N-Acetylcysteine and Divalent Metal Ions in Aqueous Solutions, *J. Chem. Eng. Data* 2014, 59, 1661–1666 (2014)

## Nanofibers of titanium phosphate modified by “green” silver nanoparticles as a perspective antibacterial nanocomposites

T. Hubetska<sup>1, 2 \*</sup>, O. Khainakova<sup>3</sup>, B. Cabal<sup>1</sup>, N. Kobylinska<sup>1</sup>, A. Fernández<sup>1</sup>

1) Nanomaterials and Nanotechnology Research Center (CINN-CSIC), University of Oviedo (UO), Spain

2) A.V. Dumansky Institute of Colloid and Water Chemistry, National Academy of Science of Ukraine, Ukraine

3) University of Oviedo-CINN, Spain

\* thubetska AT gmail.com

Nanofibres have attracted a great deal of attention over the last two decades due to their unique properties, which make them appealing for use in various areas of medicine. Typically, different polymers can be easily fabricated with a fibrous morphology. However, these nanofibres generally perform poorly in adverse conditions such as high temperatures, irradiation, scratching and erosive solvents. A good alternative could be fibrous titanium phosphate (TiP) nanomaterials, which are chemically stable, low toxicity, biocompatible, formable, corrosion resistant, with excellent ion exchange properties for easy incorporation of target agents, e.g., antibacterial compounds

The aim of this work was to obtain the  $\pi$ -phase of crystalline titanium phosphate ( $\pi$ -TiP) in a fibrous form to use as a support for 'green' synthesized silver nanoparticles (AgNPs) in various antibacterial applications. The  $\pi$ -TiP solids were prepared via the sol-gel method followed by microwave-assisted hydrothermal treatment using the reaction between a titanium chloride (2M  $\text{TiCl}_4$ ) and a phosphoric acid (1.6M  $\text{H}_3\text{PO}_4$ ). Structural and microscopic studies, using X-ray diffraction, transmission (TEM), and scanning (SEM) electron microscopy data, confirm the formation of fibrous  $\pi$ -phases and their enrichment, with an average particle size of around 100 nm.

The affinity of the  $\pi$ -TiP nanoparticles toward antibacterial agents such as AgNPs was studied in static conditions. Previously, the series of AgNPs solutions was obtained using Melissa extracts (70% alcohol) and silver(I) acetate (AgAc) solution with various concentrations (1, 5, and 10 mM). The variables affecting the synthesis of AgNPs, including precursor concentration, reducing extract concentration, temperature, and reaction time, were investigated. TEM images demonstrated that the obtained AgNPs were spherical in shape with an average size of 10 to 15 nm. The as-synthesized AgNPs were incorporated into the  $\pi$ -TiP nanofibers. The successful formation and stability of the  $\pi$ -TiP/AgNPs nanocomposites were confirmed by various techniques. TEM images of  $\pi$ -TiP/AgNPs nanocomposites indicate uniform distribution of monodisperse AgNPs without changes in the starting size. Also, FTIR spectroscopy and TGA indicated the significant contribution of polyphenol extract components to the chemical composition of  $\pi$ -TiP/AgNPs nanocomposites.

Finally, the antibacterial tests showed that  $\pi$ -TiP/AgNPs nanosystems have excellent antibacterial activity against gram-negative (*Escherichia coli*) and gram-positive (*Staphylococcus aureus*) bacteria. The  $\pi$ -TiP/AgNPs nanofibers are effective for the prohibition of the growth of different bacteria and, therefore, are expected to be used as stable antibacterial materials.

---

**KEYWORDS:** Titanium phosphate, Nanofibers, Silver nanoparticles, Antibacterial nanocomposite

---

**ACKNOWLEDGEMENTS:** This study was supported by CSIC grants “UCRANIA DOCTORES 2022”. CINN-UNIOVI thanks for the financial support Spanish MINECO MCI-21-PID2020- 113558RB-C41, and PID2020- 119130 GB-I00.

## Structural and defect evolution in nanostructured spinel ceramics under phase modification

Y. Kostiv<sup>1\*</sup>, H. Klym<sup>1</sup>

*1) Lviv Polytechnic National University, Ukraine*

\* yura.kostiv AT gmail.com

Spinel-type ceramics have attracted considerable attention due to their wide range of functional applications. In particular,  $\text{Cu}_{0.1}\text{Ni}_{0.8}\text{Co}_{0.2}\text{Mn}_{1.9}\text{O}_4$  ceramics exhibit pronounced temperature sensitivity, making them suitable for negative temperature coefficient (NTC) thermistors, high-precision temperature sensors, and inrush current limiting devices [1].

The sintering process plays a key role in determining both the structural and electrical properties of these materials, as it governs phase composition in the bulk and near-surface regions. A reduction in the NiO phase fraction has been found to significantly suppress thermal aging, ensuring resistance stability within 3%. To further improve long-term performance, chemical modification using metallic additives has been implemented. These additives, primarily located in intergranular regions, stabilize cation distribution within grains and mitigate thermally activated degradation processes. The strong correlation between structural features and thermal behavior highlights the need for advanced characterization techniques.

In this study, positron annihilation lifetime (PAL) spectroscopy was employed to investigate microstructural evolution, as it is highly sensitive to regions of reduced electron density. However, interpretation of PAL data requires careful consideration of crystallographic factors and grain boundary effects, necessitating a comprehensive analytical approach. This method provides detailed insight into defect distributions and grain-pore interactions within the ceramics [2].

Ceramic samples were prepared via controlled sintering with varying NiO content ranging from 1% to 12%. Microstructural analysis revealed that increasing NiO concentration promotes grain growth, grain coalescence, and modification of defect structures. PAL measurements showed that positron trapping rates strongly depend on NiO content. At 8% NiO, defect fragmentation enhances positron trapping efficiency, whereas at 10% an optimal balance between structural stability and defect concentration is achieved. Further increase to 12% results in excessive grain merging, reducing grain boundary density and consequently decreasing positron trapping efficiency.

These results demonstrate that the nanostructure of  $\text{Cu}_{0.1}\text{Ni}_{0.8}\text{Co}_{0.2}\text{Mn}_{1.9}\text{O}_4$  ceramics is highly sensitive to NiO phase distribution and its interaction with grain boundaries. The observed variations in positron trapping correlate with microstructural evolution and reflect the influence of thermal conditions during sintering on defect formation. It is established that a NiO content of 10% provides optimal structural stability and minimizes defect-related degradation. The combination of PAL spectroscopy with conventional characterization techniques enables a deeper understanding of ceramic behavior at the nanoscale. These findings contribute to the development of advanced spinel ceramics with improved performance for temperature-sensitive electronic applications.

---

**KEYWORDS:** Spinel ceramics, NTC thermistors, NiO phase, Free-volume defects, Positron annihilation lifetime spectroscopy

---

**ACKNOWLEDGEMENTS:** This work was supported by the Ministry of Education and Sciences of Ukraine (Project No 0125U001883).

---

### REFERENCES

- [1] Z. Song, Z. Chen, G. Du, L. Huang, J. Yin, J. Cao, Y. Guo, Research progress on negative temperature coefficient thermistors. *Journal of Materials Science: Materials in Electronics*, 36(11), 688 (2025).
- [2] F. Constantin, M. Petruneac, M. Focsaneanu, Positron annihilation spectroscopy studies of implanted polymer membranes. *Polymers for Advanced Technologies*, 32(1), 241-247 (2021).

## Optical characterization of carbon nanodots produced from coffee waste via green synthesis using visible spectroscopy and Rayleigh scattering

S. Akkuş<sup>1</sup>\*, Y. Ozturk<sup>2</sup>

1) Ege University, Turkey

2) Department of Electrical and Electronics Engineering, Faculty of Engineering, Ege University, İzmir, Turkey

\* sareakkus123 AT gmail.com

Carbon nanodots (CDs) are emerging as promising nanomaterials for bioimaging, sensing, and photocatalysis due to their exceptional photoluminescence, biocompatibility, and chemical stability [1]. Their quantum-confined optical properties and low cytotoxicity make them attractive alternatives to conventional semiconductor quantum dots and organic dyes. However, nanoscale verification of CDs typically relies on expensive electron microscopy techniques such as TEM and AFM, limiting accessibility for researchers with constrained budgets [2]. The development of cost-effective optical methods capable of supporting nanoscale characterization remains an important challenge in sustainable nanomaterial research.

Here we show that standard visible spectroscopy (450-850 nm), when systematically coupled with Rayleigh scattering analysis, can provide a complementary and cost-effective approach for supporting nanoscale verification of CDs synthesized from coffee waste—an abundant biomass source—via green thermal carbonization at 220°C. Coffee grounds were first thermally treated in an oven at 220°C, followed by aqueous extraction. The obtained suspension was purified by high-speed centrifugation (12,000 rpm, 25 min) to remove macroscopic residues and then filtered through a 0.22 µm membrane to eliminate larger aggregates, improving colloidal stability. We obtained stable colloidal solutions exhibiting blue/turquoise photoluminescence under 365 nm UV excitation, qualitatively indicating optical behavior characteristic of carbon nanodots [3].

Quantitative Beer-Lambert analysis of systematic dilution series (1:100 to 1:1000) using an Ocean Optics spectrometer with quartz cuvette in 180° transmission geometry yielded high optical linearity ( $RZ = 0.9917$  at 480 nm), demonstrating colloidal stability and potential for concentration-dependent optical sensing applications. In addition, we applied the classical Rayleigh scattering model ( $I \propto 1/\lambda^4$ ) to optical extinction data in the long-wavelength region (600-800 nm), where absorption contributions are expected to be lower and scattering effects become more relevant [4]. High correlations ( $RZ > 0.95$ ) obtained across all concentrations support the interpretation that the particles responsible for optical extinction are substantially smaller than the incident wavelength, consistent with nanodot-like morphology without relying solely on electron microscopy.

Our results suggest that visible spectroscopy, combined with mathematical modeling, may serve as a useful complementary method to electron microscopy for supporting nanoscale verification. This approach can make CD synthesis validation more accessible for laboratories lacking expensive facilities, contributing to sustainable nanomaterial development from waste streams [5]. The high Beer-Lambert linearity indicates suitability for optical sensing, while the observed photoluminescence suggests potential for photocatalytic and bioimaging-related applications.

---

**KEYWORDS:** Carbon nanodots, Green synthesis, Rayleigh scattering, Visible spectroscopy, Coffee waste valorization

---

### REFERENCES

- [1] S. Y. Lim, W. Shen, Z. Gao, "Carbon quantum dots and their applications", *Chem. Soc. Rev.*, 44, 362-381 (2015).
- [2] Y. Wang, A. Hu, "Carbon quantum dots: synthesis, properties and applications", *J. Mater. Chem. C*, 2, 6921-6939 (2014).
- [3] Y. P. Sun, B. Zhou, Y. Lin, W. Wang, K. S. Fernando, P. Pathak, M. J. Meziani, B. A. Harruff, X. Wang, H. Wang, P. G. Luo, H. Yang, M. E. Kose, B. Chen, L. M. Veca, S. Y. Xie, "Quantum-sized carbon dots for bright and colorful photoluminescence", *J. Am. Chem. Soc.*, 128, 7756-7757 (2006).
- [4] C. F. Bohren, D. R. Huffman, "Absorption and scattering of light by small particles", Wiley-VCH, (2008).
- [5] M. M. Titirici, R. J. White, N. Brun, V. L. Budarin, D. S. Su, F. del Monte, J. H. Clark, M. J. MacLachlan, "Sustainable carbon materials", *Chem. Soc. Rev.*, 44, 250-290 (2015).

## Fabrication and characterization of ceramic thick-film nanostructures for sensor applications

H. Klym<sup>1</sup>\*, I. Hadzaman<sup>2</sup>

1) Lviv Polytechnic National University, Ukraine

2) Drohobych Ivan Franko State Pedagogical University, Ukraine

\* klymha AT yahoo.com

The use of thick-film ceramic materials based on mixed transition-metal manganite systems, combined with humidity-sensitive nanostructured MgAl<sub>2</sub>O<sub>4</sub> ceramics, is a promising approach for developing multifunctional electroceramic sensors [1]. These materials enable simultaneous detection of temperature and humidity due to their tailored electrical and structural properties [2]. This study focuses on the fabrication and structural characterization of thick-film nanostructures with dual sensitivity.

The investigated systems include spinel-structured manganites with different conductivity types: Cu<sub>0.1</sub>Ni<sub>0.8</sub>Co<sub>0.2</sub>Mn<sub>1.9</sub>O<sub>4</sub> (p-type), Cu<sub>0.1</sub>Ni<sub>0.1</sub>Co<sub>1.6</sub>Mn<sub>1.2</sub>O<sub>4</sub> (p<sup>+</sup>-type), and dielectric MgAl<sub>2</sub>O<sub>4</sub> (i-type). These materials were selected for their structural compatibility and ability to form stable multilayer architectures. Humidity-sensitive layers were deposited onto pre-formed temperature-sensitive films, enabling integration of different sensing functions within a single device.

Various multilayer configurations, including p-p<sup>+</sup>, p-p<sup>+</sup>-p, and integrated p-i-p<sup>+</sup> structures, were successfully fabricated within a single technological cycle. This approach simplifies processing and ensures reproducibility while allowing functional combination of temperature and humidity sensing elements.

Microstructural analysis shows that MgAl<sub>2</sub>O<sub>4</sub> humidity-sensitive films possess a porous structure distinct from the Al<sub>2</sub>O<sub>3</sub> substrate with Ag electrodes. The films contain fine pores that facilitate water vapor diffusion and capillary condensation at the nanoscale. Larger macropores enhance moisture transport from the environment into the bulk material, improving sensor response.

In contrast, Cu<sub>0.1</sub>Ni<sub>0.8</sub>Co<sub>0.2</sub>Mn<sub>1.9</sub>O<sub>4</sub> films exhibit a higher concentration of clustered macropores. This structural feature is consistent with that of bulk ceramics of the same composition, indicating that bulk microstructural characteristics are preserved in thick-film form. The use of spinel-structured ceramics ensures good interlayer adhesion, structural stability, and dense interfaces within multilayer systems. Controlled porosity and compatible crystal structures contribute to stable electrical behavior and improved sensor performance. Overall, the results demonstrate that manganite-based and spinel-structured ceramic thick films are highly suitable for integrated temperature and humidity sensors. Their tunable electrical properties and engineered porosity enable the development of compact, reliable, and multifunctional sensing devices for environmental monitoring applications.

---

**KEYWORDS:** Thick-film ceramics, Spinel manganites, MgAl<sub>2</sub>O<sub>4</sub> nanostructures, Humidity sensors, Temperature sensors

---

**ACKNOWLEDGEMENTS:** This work was supported by the Ministry of Education and Sciences of Ukraine (Project No 0125U001883).

### REFERENCES

- [1] Y. Ou, X. Liao, S. Chen, X. Liu, R. Li, Y. Chen, .. & Luo, J. (2026). Systematic cation engineering in spinel ferrites (MFe<sub>2</sub>O<sub>4</sub>, M= Fe, Co, Ni, Zn) for sub-ppm acetone sensing in non-invasive breath-based diabetes diagnosis. *Journal of Alloys and Compounds*, 186324.
- [2] L. Almulla, M. Mariello, C.M. Proctor, High Dynamic Range Thin-Film Resistive Flow Sensors for Monitoring Diverse Biofluids. *Advanced Functional Materials*, 36(6), e10372 (2026).

## Heat transfer analysis of SWCNT-reinforced polymer-based refractory nanocomposites

I. Zhydenko<sup>1\*</sup>, H. Klym<sup>1</sup>, K. Ivan<sup>2</sup>, D. Chalyy<sup>3</sup>

1) Lviv Polytechnic National University, Ukraine

2) Ivan Franko National University of Lviv, Ukraine

3) Lviv State University of Life Safety, Ukraine

\* i.zhydenko AT i.ua

Refractory nanocomposites are advanced materials characterized by high thermal resistance, chemical stability, and strong mechanical performance, making them suitable for extreme environments such as aerospace, energy systems, and metallurgy. Among them, carbon nanotube (CNT)-reinforced composites have attracted significant interest due to the exceptional thermal, electrical, and mechanical properties of CNTs, which enhance the performance of conventional refractory matrices [1,2].

This study investigates the thermal behavior of refractory nanocomposites containing 0.5% single-walled carbon nanotubes (SWCNTs) using an automated measurement approach. The experiments are based on a steady-state heat flow method, where thermal conductivity is evaluated by analyzing the temperature gradient along cylindrical samples subjected to controlled heating and cooling cycles. The setup includes a resistive heater, two thermocouples, and a thermal shielding system to ensure stable conditions. Data acquisition and real-time monitoring are performed using LabVIEW software.

The results show that SWCNT incorporation significantly improves the thermal properties of the polymer matrix. Infrared thermography reveals a well-defined temperature gradient and efficient heat distribution. Samples with a 2-hour dispersion time demonstrate better thermal stability compared to those with 1-hour dispersion. This is reflected in a more uniform temperature field and reduced thermal fluctuations. The maximum temperature difference reaches 55°C for the 2-hour samples, while it is about 50°C for the 1-hour samples. Overall, increasing dispersion time by one hour improves heat transfer efficiency and enhances fire resistance by approximately 15%.

The automated measurement system minimizes experimental errors by ensuring precise control of testing conditions. Potential inaccuracies caused by heater displacement or improper thermocouple positioning are reduced through careful system design and calibration. The use of high-precision sensors and a LabVIEW-based acquisition system ensures reliable and reproducible results.

Thermal imaging confirms that SWCNT-reinforced nanocomposites provide more uniform heat distribution, reducing localized thermal stress and improving material durability. Enhanced thermal conductivity and stability indicate strong potential for applications requiring high-temperature resistance, including aerospace structures, fire-resistant coatings, and industrial sensing systems. Overall, the study demonstrates that SWCNT-reinforced refractory nanocomposites are promising materials for high-temperature applications. The proposed automated methodology offers an efficient and reliable approach for evaluating thermal properties and supports further development of advanced refractory materials.

---

**KEYWORDS:** Refractory nanocomposites, Carbon nanotubes, Thermal conductivity, Steady-state heat flow method, Automated measurement system

---

**ACKNOWLEDGEMENTS:** This work was supported by the Ministry of Education and Sciences of Ukraine (Project No 0125U001883).

---

### REFERENCES

- [1] K.P. Socrates, A. Vasanthanathan, The Perspectives, Synthesis, and Archives of CNT-Based Carbon Fiber-Reinforced Composites: A State-Of-The-Art Review. *Polymer-Plastics Technology and Materials*, 65(5-6), 601-618 (2026).
- [2] S. Kumar, V.K. Mahakur, D.K. Mishra, N. Kumar, N.K. Chougule, Performances and decision framework of CNT-infused bio-based hybrid composites for lightweight smart structures. *Scientific Reports* (2026).

## Rutin-loaded hydrogels for skin repair: Antioxidant and antimicrobial properties

L. Sukhodub<sup>1</sup>\*, N. Bozhko<sup>1</sup>, M. Kumeda<sup>1</sup>, O. Korenkov<sup>1</sup>, L. Sukhodub<sup>1</sup>

1) Sumy State University, Ukraine

\* l.sukhodub AT gmail.com

The development of biomaterials for the treatment of skin defects, including burns, ulcers, and other wounds, remains a highly relevant area of modern regenerative medicine. Skin serves as an essential barrier and protective function, and its damage may lead to serious complications, including infection and fluid loss [1]. The effectiveness of biomaterials for skin repair depends on their composition and structure [2]. Among the most promising materials for the treatment of skin defects are hydrogels, owing to their high biocompatibility, ability to maintain an optimal moist wound environment, and capacity to incorporate bioactive compounds and therapeutic agents. Their strong adhesion to the skin surface also makes them suitable for treating wounds of various shapes. Among biopolymers, gelatin, collagen, chitosan, fibrin, and alginates are widely used for biomaterial fabrication because of their favorable regenerative properties, ability to promote cell adhesion, and support for new tissue formation. In recent years, research has increasingly focused on the development of intelligent biomaterials capable of actively modulating immune responses and cellular metabolism.

It has been shown that biomaterial properties such as hydrophilicity, porosity, and the presence of immobilized inorganic nanoparticles significantly affect the rate of wound recovery and regeneration [3]. It is established that wound healing is associated with increased levels of reactive oxygen species (ROS), which degrade extracellular matrix (ECM) proteins and may delay the healing process [4]. Therefore, the use of antioxidants is of particular interest. Among them, rutin is a flavonoid that reduces oxidative stress in wounds, improves microcirculation, stimulates tissue regeneration, exhibits moderate antibacterial activity, prevents lipid peroxidation, and protects proteins and DNA [5].

The aim of this study is to determine the antioxidant and antimicrobial properties of rutin incorporated into an alginate-gelatin matrix with immobilized inorganic particles.

Alginate-gelatin wound dressings doped with nanosized calcium-deficient hydroxyapatite particles were synthesized. Rutin was introduced into the matrix in two ways: i) by adding it to the working suspension during synthesis (at a concentration of 4% of the volume of the working mixture); ii) by saturating the finished biomaterial with an aqueous 4% solution of rutin. The results showed that the antioxidant activity (AOA) of the prepared composites was 94% with rutin introduced during synthesis and 92% with saturation. The addition of rutin increases the antimicrobial activity: The zone of bacterial growth inhibition (ZOI) is 23 mm, compared to the control, where the ZOI is 20 mm (sample size - 11 mm).

Based on the obtained physicochemical and biological characteristics, the developed materials show considerable promise for the treatment of inflammatory skin wounds and are currently undergoing further studies.

---

**KEYWORDS:** Wound healing, Hydrogels, Antioxidant activity, Inorganic particles, Skin regeneration

---

**ACKNOWLEDGEMENTS:** The Ministry of Education and Science of Ukraine financially supported the research.

---

### REFERENCES

- [1] Y. Xiong *et al.*, "The role of the immune microenvironment in bone, cartilage, and soft tissue regeneration: from mechanism to therapeutic opportunity," 2022. doi: 10.1186/s40779-022-00426-8.
- [2] Y. Wang *et al.*, "3D bioprinting for tendon-bone interface regeneration," 2025. doi: 10.36922/ijb.8411.
- [3] L. Sukhodub, M. Kumeda, L. Sukhodub, V. Bielai, and M. Lyndin, "Metal ions doping effect on the physicochemical, antimicrobial, and wound healing profiles of alginate-based composite," *Carbohydr. Polym.*, vol. 304, 2023, doi: 10.1016/j.carbpol.2022.120486.
- [4] P. Le Thi *et al.*, "In situ forming and reactive oxygen species-scavenging gelatin hydrogels for enhancing wound healing efficacy," *Acta Biomater.*, vol. 103, 2020, doi: 10.1016/j.actbio.2019.12.009.
- [5] L. Y. Chen *et al.*, "Effects of rutin on wound healing in hyperglycemic rats," *Antioxidants*, vol. 9, no. 11, 2020, doi: 10.3390/antiox9111122.

## Aligned PCL electrospun membranes for nerve guidance conduits

V. Kulibaba<sup>1\*</sup>, Y. Husak<sup>1</sup>, I. Bulyha<sup>2</sup>, A. Liutyi<sup>3</sup>, O. Solodovnyk<sup>3</sup>, I. Yanko<sup>1</sup>, S. Dmytruk<sup>1</sup>, S. Kyrlyenko<sup>1</sup>, V. Korniienko<sup>4,5</sup>, M. Pogorielov<sup>5,4</sup>

1) Biomedical Research Center, Academic and Research Medical Institute, Sumy State University, Sumy, Ukraine

2) Sumy State University, Ukraine

3) Sumy State University, Sumy, Ukraine

4) University of Latvia, Riga, Latvia

5) Biomedical Research Center, Medical Institute, Sumy State University, Sumy, Ukraine

\* bik.kylibaba AT gmail.com

Peripheral nerve injuries are a common problem in medicine due to their high prevalence, diverse etiologies, and the incomplete functional recovery [1]. Artificial nerve guidance conduits (NGCs) represent an advanced strategy for the treatment of extensive peripheral nerve injuries, and their development remains a major focus in regenerative medicine [2,3]. Electrospun polycaprolactone (PCL) membranes considered among the most promising candidates for this purpose [4]. PCL exhibits favorable mechanical strength and elongation at break [5]. But, traditional randomly-oriented electrospun PCL membranes do not allow to support directed axonal regeneration by guiding nerve growth. The aim of the study was to develop aligned electrospun PCL membranes with properties suitable for guiding nerve regeneration.

PCL was dissolved in a 3:1 chloroform/dimethylformamide (CHL/DMF) mixture under continuous stirring with a magnetic stirrer for 2 h. Electrospinning was carried out at an applied voltage of 15-21 kV using G-22 needles. The distance between the needle tip and the drum collector maintained at 13-16 cm. The collector rotation speed was set to 600 rounds per minute (RPM) for the control sample ( $S_1$ ) and 1000 RPM ( $S_2$ ), 2000 RPM ( $S_3$ ), and 3000 rpm ( $S_4$ ) for the experimental ones. The structural features and morphology of the obtained membranes were evaluated using scanning electron microscopy (SEM) (Hitachi TM-3000, Japan) operated at an accelerating voltage of 15 kV in backscattered electron (BSE) mode. Morphometric analysis of the SEM images was performed using ImageJ software.

All PCL membrane samples exhibited a fibrous morphology; however, their structural characteristics varied depending on the collector rotation speed. In general, increasing the rotation speed resulted in a reduction in fiber diameter, from  $0.39 \pm 0.13 \mu\text{m}$  in  $S_1$  to  $0.051 \pm 0.05 \mu\text{m}$  in  $S_4$ . At the same time, the membranes showed differences in fiber thickness uniformity, with the highest uniformity observed for  $S_2$ , while  $S_3$  and  $S_4$  demonstrated a broader distribution of fiber diameters. The analysis of fiber orientation also demonstrated clear structural differences between the samples.  $S_2$  showed the most pronounced unidirectional fiber alignment, as confirmed by the lowest coefficient of variation in fiber orientation angles.  $S_4$  exhibited a partially ordered structure, whereas  $S_3$  showed weak anisotropy. In contrast,  $S_1$  demonstrated a predominantly random fiber arrangement.

Overall, increasing the collector rotation speed provided effective control over the morphology of electrospun PCL membranes, including fiber diameter, and fiber orientation. Among the fabricated samples,  $S_2$  demonstrated the most favorable combination of structural features, particularly improved fiber uniformity and pronounced unidirectional alignment. These characteristics make  $S_2$  the most promising membrane configuration for applications requiring guided tissue regeneration.

**KEYWORDS:** Electrospinning, Aligned nanofibers, NGCs, PCL nanofibers

**ACKNOWLEDGEMENTS:** This research was supported by the Ministry of Education and Science of Ukraine (Projects No. 0126U000870, 0124U000637, 0124U000552).

### REFERENCES

- [1] M. Nadi, W. Dabbas, J.M. Das. Peripheral Nerve Injury [Internet]. Treasure Island (FL): StatPearls Publishing; 2026 Jan-. [updated 2026 Feb 15; cited 2026 Apr 29]. Available from: <https://www.ncbi.nlm.nih.gov/books/NBK549848/>
- [2] C. Zheng, Z. Yang, S. Chen, F. Zhang, Z. Rao, C. Zhao, D. Quan, Y. Bai, J. Shen. Nanofibrous nerve guidance conduits decorated with decellularized matrix hydrogel facilitate peripheral nerve injury repair. *Theranostics*. 2021;11(6):2917-2931. doi:10.7150/thno.50825.
- [3] L. Zhu, S. Jia, T. Liu, L. Yan, D. Huang, Z. Wang, S. Chen, Z. Zhang, W. Zeng, Y. Zhang, H. Yang, D. Hao. Aligned PCL fiber conduits immobilized with nerve growth factor gradients enhance and direct sciatic nerve regeneration. *Adv Funct Mater*. 2020;30(39):2002610. doi:10.1002/adfm.202002610.
- [4] Y. Guo, X. Wang, Y. Shen, K. Dong, L. Shen, A.A. Alzalab. Research progress, models and simulation of electrospinning technology: a review. *J Mater Sci*. 2022;57(1):58-104. doi:10.1007/s10853-021-06575-w.
- [5] Q. Zhao, S.B. Lu, Q. Quan, H.Y. Meng, B. Chang, G.B. Liu, X.Q. Cheng, H. Tang, Y. Wang, J. Peng. Aligned fibers enhance nerve guide conduits when bridging peripheral nerve defects focused on early repair stage. *Neural Regen Res*. 2019;14(5):903-910. doi:10.4103/1673-5374.249239.

## Mechanical response of irradiated niobium-tin alloy with nanoscale $A_{15}$ -phase precipitates: Phase-field modeling

O. Shchokotova<sup>1</sup>\*, D. Kharchenko<sup>1</sup>, V. Kharchenko<sup>1</sup>

*1) Institute of Applied Physics National Academy of Sciences of Ukraine, Ukraine*

\* shchokotova.o AT gmail.com

Niobium-Tin alloys containing nanoscale precipitates of the  $A_{15}$  intermetallic phase attract considerable interest as advanced structural and functional materials due to their high mechanical stability, radiation resistance, and potential applications in extreme environments. In the present work, a phase-field approach is developed to investigate the mechanical response of two-phase Nb-20 at.% Sn alloys containing nanoscale  $A_{15}$  precipitates before and after irradiation.

The model combines thermodynamic free-energy formalism with nonlinear elasticity theory and explicitly accounts for the coupled evolution of local composition fields, vacancy concentration, and elastic displacement fields. Radiation-induced nonequilibrium vacancies are incorporated through defect-strain coupling terms, while elastic mismatch between the matrix and  $A_{15}$  precipitates is described using composition-dependent elastic moduli and periodic nonlinear shear energy. Dynamic evolution of the elastic fields is described by the lattice momentum equation coupled with phase-field kinetic equations.

Numerical simulations were performed for both pre-irradiated and post-irradiated alloys with nanosized precipitates of  $A_{15}$ . Mechanical behavior was investigated under monotonic shear loading, cyclic shear deformation, and uniaxial compression/tension. The simulations demonstrate that irradiation leads to a pronounced increase in yield strength and ultimate strength, indicating radiation-induced hardening of the Nb-Sn alloy. Under shear loading, the yield stress increases, while the ultimate strength increases from after irradiation. Similar strengthening effects are observed under compressive and tensile loading.

Spatial analysis of elastic fields reveals that plastic deformation is governed by the nucleation and propagation of slip lines associated with pairs of edge dislocations. These defects preferentially nucleate in the softer Nb matrix and are strongly influenced by nanoscale  $A_{15}$  precipitates, which act as barriers for dislocation motion and promote stress localization. Under cyclic loading, hysteresis loops and residual stresses are observed, with irradiated samples exhibiting reduced plastic strain accumulation and enhanced cyclic hardening.

The obtained results demonstrate that irradiation-induced defect structures together with nanoscale  $A_{15}$  precipitates substantially modify the deformation mechanisms in Nb-Sn alloys by suppressing dislocation mobility and increasing resistance to plastic flow. The developed approach provides a useful framework for predicting the mechanical performance of radiation-resistant nanostructured superconducting and structural materials.

---

**KEYWORDS:** Numerical modeling, Deformation, Elastic fields, Strength

---

**ACKNOWLEDGEMENTS:** The work was supported by the Ministry of Education and Science of Ukraine (grant No. 0124U000551)

## Theoretical analysis of the geometry of graphene scrolls

J. Aljedani<sup>1</sup> \*

*1) King Abdulaziz University, Saudi Arabia*

\* jaljedani AT kau.edu.sa

The global market is experiencing an unprecedented surge in foldable electronics innovations. Among the materials enabling this technological leap, graphene has emerged as a promising material, owing to its inherent flexibility, bendability, and elasticity, positioning it as a key component in the fabrication of these devices. This work proposes a theoretical model to advance our knowledge of the mechanisms of graphene scrolling. Through this model, we study the minimum length of graphene required to form a particular number of scrolls by examining the energy cost. The model takes into account the bending rigidity of graphene and the van der Waals (vdW) interaction energy between carbon atoms within the graphene sheet. The Lennard-Jones potential is employed within the model to evaluate the vdW interaction energy arising from the graphene interlayer interactions during the scrolling formation. Then, the scrolling conformation of graphene is presented as parametric solutions derived from variational techniques adopting the Ritz method. The findings of the proposed model are subsequently compared with experimental data reported in the literature, and the comparison demonstrates good agreement in terms of the inner and outer radii of the scroll, number of coils, and total length. The model predicts that the total length of graphene scrolling structures containing one to five coils varies from 6.0 to 70.7 nm, depending on both the number of coils and the model parameters. For example, the total length of a three-coil graphene scroll with a bending rigidity of 1.2 eV [1], is calculated to be 27.5 nm, which lies well within the experimentally reported range of 18.1-36.7 nm [2]. The theoretical approach presented here holds the potential to significantly reduce the time and cost associated with trial-and-error experiments in characterizing graphene scrolling behavior, with direct implications for the design of next-generation foldable electronic devices.

---

**KEYWORDS:** Graphene, Mathematical model, Variational calculus, Scrolling conformation, Foldable electronics

---

**ACKNOWLEDGEMENTS:** The research was funded by the Deanship of Scientific Research (DSR) at King Abdulaziz University, Jeddah, Saudi Arabia. The authors, therefore, acknowledge with thanks DSR for technical and financial support.

---

### REFERENCES

- [1] R. Nicklow, N. Wakabayashi, H.G. Smith, Lattice dynamics of pyrolytic graphite. *Physical Review B*, 5(12), 4951 (1972).
- [2] A.V. Savin, E.A. Korznikova, S.V. Dmitriev, Scroll configurations of carbon nanoribbons. *Physical Review B*, 92(3), 035412 (2015).

## Förster resonance energy transfer in restricted geometry

A. Schlichtholz<sup>1</sup>\*, A. Synak<sup>1</sup>, P. Bojarski<sup>1</sup>, K. Schlichtholz<sup>1</sup>, L. Kułak<sup>2</sup>

1) University of Gdansk, Poland

2) Gdańsk University of Technology, Poland

\* agnieszka.schlichtholz AT phdstud.ug.edu.pl

Non-radiative energy transfer in luminescent systems based on the dipole-dipole interaction mechanism proposed by Förster [1] has been widely employed as a nanoscale spectroscopic ruler. This approach provides valuable information on the conformational distributions of biologically active macromolecules and has found applications in bioimaging analysis, evaluation of targeted drug therapies, biosensing, and antenna systems. Particularly intriguing are studies of Förster Resonance Energy Transfer (FRET) in spatially confined systems. In such cases, theoretical descriptions developed for macroscopic systems cannot be applied directly. Here, we present a description of FRET in systems of limited volume and well-defined geometry, specifically spherical [2,3] and cylindrical structures. A theoretical model describing the dependence of FRET on system parameters, including spatial dimensions, number of fluorophores, and the properties of a specific donor-acceptor pair, has been developed and presented, and Monte Carlo simulations were performed to investigate the energy transfer behavior.

---

**KEYWORDS:** Förster resonance energy transfer, Restricted geometry, Spherical nanostructures, Cylindrical nanostructures, Monte Carlo simulations

---

### REFERENCES

- [1] T. Förster, "Zwischenmolekulare Energiewanderung Und Fluoreszenz", *Annalen der Physik*, 437 (1-2), 55-75 (1948)
- [2] A. Synak, L. Kułak, P. Bojarski, A. Schlichtholz, "Förster Energy Transfer in Core-Shell Nanoparticles: Theoretical Model and Monte Carlo Study". *J. Phys. Chem. C* 125 (33), 18517-18525, (2021)
- [3] A. Schlichtholz, L. Kułak, K. Schlichtholz, P. Bojarski, "Model of Energy Transfer within the Shell Layer of Core-Shell Nanoparticle" *TJ. Phys. Chem. C*, 129(39), 17599-17606 (2025)

## Advanced nanocomposites based on fibers titanium phosphate with "green" AgNPs for multifunctional environmental applications

T. Hubetska<sup>1, 2 \*</sup>, S. González-Fernández<sup>1</sup>, B. Cabal<sup>1</sup>, N. Kobylinska<sup>1</sup>, A. Fernández<sup>1</sup>

1) Nanomaterials and Nanotechnology Research Center (CINN-CSIC), University of Oviedo (UO), Spain

2) A.V. Dumansky Institute of Colloid and Water Chemistry, National Academy of Science of Ukraine, Ukraine

\* thubetska AT gmail.com

Hazardous materials such as organic, inorganic, radioactive, biological, and physical are found in environmental water. The environmental remediation of wastewater has remained a paramount concern for researchers over the past few decades. The solution to this problem may be the development of multifunctional advanced materials. Among various inorganic frameworks, fibrous titanium phosphate (TiP) stands out as a support matrix due to its high surface area, ion-exchange capacity, and stability. These structural attributes make it an ideal matrix for the impregnation of functional guest species, such as silver nanoparticles (AgNPs), which are renowned for their potent biocidal and remediation properties.

In this work, an effective and cheap inorganic nanocomposite based on fibrous titanium phosphate with embedded AgNPs (TiP@AgNPs) was first developed for potential multifunctional environmental applications. The AgNPs were prepared by "green" synthesis using CH<sub>3</sub>COOAg solution and *Melissa officinalis* extract (EtOH, 70 %). The biosynthesized AgNPs were characterized through a series of instrumental methods. The UV-Vis spectrum of the AgNPs exhibited a  $\lambda_{max}$  at 425 nm. The size of biosynthesized AgNPs is estimated to be ~ 15-18 nm according to the TEM method. Additionally, the as-prepared AgNPs exhibited nucleoprotective properties due to the formation of a 'core-shell' structure, which prevented the aggregation of the resulting nanoparticles. As expected, AgNPs could be stored for more than 1 year at room temperature. The TiP@AgNPs nanocomposite was prepared by in-situ treatment of nanofibres with biosynthesized AgNPs. TEM data of TiP@AgNPs show that the AgNPs are distributed uniformly and monodispersely across the surface of fibres. The TiP@AgNPs nanocomposite exhibited potent antibacterial activity against both Gram-positive (*S. aureus*) and Gram-negative (*E. coli*). The Gram-negative strain proved more susceptible, with minimum inhibitory concentration and minimum bactericidal concentration of 0.5-1.0 mg/mL and 1.0 mg/mL, respectively. Furthermore, when utilizing TiP@AgNPs as sensors for Hg<sup>2+</sup> ions detection in both double-distilled and deionised waters, the limits of detection (LOD) were determined to be 0.030  $\mu$ M and 0.025  $\mu$ M, respectively, within a wide linear range (0.05-2.00  $\mu$ M). Thus, the as-prepared nanocomposite demonstrates multifunctionality as a highly sensitive sensor for Hg<sup>2+</sup> ions detection in various water matrixes and a potent antibacterial agent.

**KEYWORDS:** Fibrous titanium phosphate, Silver nanoparticles, Green synthesis, Antibacterial activity, Hg 2+

**ACKNOWLEDGEMENTS:** This study was supported by CSIC grants "UCRANIA DOCTORES 2022". CINN-UNIOVI thanks for the financial support Spanish MINECO MCI-21-PID2020- 113558RB-C41, and PID2020- 119130 GB-I00.

# Track 2

MXenes: Physics, Chemistry, and Applications

## From flakes to functions: Design-driven MXene platforms for energy and bio-interfaces

M. Namvari<sup>1</sup> \*

1) Sabanci University, Turkey

\* mina.namvari AT sabanciuniv.edu

Two-dimensional MXenes have rapidly evolved from laboratory curiosities to versatile platforms for multifunctional devices, yet translating their exceptional intrinsic properties into robust technologies remains a central challenge. In this invited talk, I will present a design-driven approach to MXene-based materials, spanning synthesis, scalable assembly, and integration into functional architectures for energy storage, tissue engineering, cancer therapy, and anti-icing/deicing applications.

I will first discuss how rational selection of MXene chemistry, flake morphology, and interface engineering enables high-performance, flexible, and environmentally benign nanocomposites for electromagnetic shielding and next-generation energy storage, highlighting our recent work on MXene-cellulose nanofiber and MXene-polyimide systems. Building on these concepts, I will then show how structure-property control-via electrophoretic deposition and tailored surface terminations-can be leveraged to create mechanically robust, conformal coatings and layered architectures, offering a pathway from batch synthesis to scalable, industry-relevant manufacturing. I will further explain how surface modification of MXene tunes its compatibility with polymer matrices and enhances supercapacitance, providing guidelines for optimizing electrochemical performance. Finally, I will outline emerging opportunities where MXene’s unique combination of metallic conductivity, hydrophilicity, and photothermal/electrothermal responsiveness is harnessed for cancer therapy and anti-icing/deicing coatings, pointing to strategies that couple multiphase design with multifunctionality to address reliability, stability, and safety requirements in real-world environments.

By connecting fundamental design rules with application-specific constraints, this talk aims to provide a coherent framework for engineering MXene-based systems that bridge the gap between laboratory prototypes and practical devices.

---

**KEYWORDS:** MXene, Surface modification, Tissue engineering, Electrode, Cancer therapy

---

**ACKNOWLEDGEMENTS:** This work was financially supported by Sabanci University Nanotechnology Research and Application Center (SUNUM), and FLAG-ERA Grant [GRAPHOCD], by the Scientific and Technological Research Council of Turkey (TUBITAK) [223N171].

---

### REFERENCES

- [1] M. Namvari\*, T. Inan, A. Altan. MXene-cellulose nanofiber composites: Towards green, multi-functional, flexible, and highly efficient electromagnetic shielding materials. *Graphene and 2D Materials* 2023, 8, 5-26 . <https://doi.org/10.1007/s41127-023-00056-4>
- [2] A. Altan, M. Namvari\*. Multifunctional, Flexible, and Mechanically Robust Polyimide-MXene Nanocomposites. *2D Materials*, 2023, 10, 042001 DOI 10.1088/2053-1583/acf327
- [3] M. Namvari\*, K. Barun. Chakrabarti. Electrophoretic Deposition of MXenes and their Composites: Towards a Scalable Approach. *Advances in Colloid and Interface Science*, 2024, 331, 103208. <https://doi.org/10.1016/j.cis.2024.103208>
- [4] A. Güngör, M. Namvari\*, A. B. Ayed, E. Erdem. Electrochemical and Defect Characterization of APTES-Functionalized Ti3C2Tx MXene for Supercapacitor Devices. *Small (INVITED)*, 2025, <https://doi.org/10.1002/sml.202505698>
- [5] M. Zahrabi, M. Altunbek, S. Çelik, M. Namvari\*, B. Koc. 3D melt electrowritten MXene-reinforced scaffolds for tissue engineering applications. *Biofabrication*, 2025, 17, 045011 DOI 10.1088/1758-5090/adf803
- [6] R. A. Ghotli, Z. Kudaş, R. Zaidi, K. B. Dönmez, Z. Çobandede, A. B. Ayed, M. Namvari, B. Alkhateab, S. Çelik, F. S. Mjalli, Y. Tülay. Inan, Mustafa Kemal Bayazit, Serap Hayat Soytaş, Nigel P. Brandon, Barun Kumar Chakrabarti. All-Vanadium Redox Flow Battery Electrodes Enhanced with Nanomaterial Catalysts via Binder-Free Electrophoretic Deposition. *ChemCatChem*, 2025 <https://doi.org/10.1002/cctc.202501280>
- [7] A. B. Ayed, M. Namvari\*. Design strategies in developing MXene-based anti-icing/deicing coatings: toward energy-efficient and durable solutions. *Advanced Composites and Hybrid Material*, 2025, 8, 410 <https://doi.org/10.1007/s42114-025-01469-w>
- [8] R. A. Ghotli, M. Namvari\*, B. Chakrabarti. Electrochemical Etching: Towards a Scalable Production of MXene. *Advanced Materials Technologies*, 2026, <https://doi.org/10.1002/admt.202501403>

## MXenes for environmental remediation: From fundamental science to sustainable solutions

S. Ramanavičius<sup>1\*</sup>, S. Ali<sup>2</sup>, A. Raveendran<sup>1</sup>, M. Sajid<sup>1</sup>, G. Paulikaite<sup>3</sup>, I. Navitski<sup>4</sup>, K. Sobol<sup>5</sup>, Š. Žukauskas<sup>6</sup>, A. Popov<sup>7</sup>, O. Gogotsi<sup>8</sup>, A. Ramanaviciene<sup>9</sup>, A. Ramanavičius<sup>10, 11</sup>

1) Department of Electrochemical Material Science, State Research Institute Center for Physical Sciences and Technology, Lithuania

2) Department of Organic Chemistry, Center for Physical Sciences and Technology (FTMC), Saulėtekio Av. 3, LT-10257 Vilnius, Lithuania, Lithuania

3) Department of Electrochemical Material Science, State Research Institute Center for Physical Sciences and Technology (Lithuania), Lithuania

4) Center for Physical Sciences and Technology (FTMC), Vilnius, Lithuania

5) NanoTechnas - Center of Nanotechnology and Materials Science, Institute of Chemistry, Faculty of Chemistry and Geosciences, Vilnius University, Naugarduko St. 24, LT-03225 Vilnius, Lithuania., Lithuania

6) Centre for Innovative Medicine, Lithuania; Center for Physical Sciences and Technology, Lithuania, Lithuania

7) NanoTechnas - Center of Nanotechnology and Materials Science, Institute of Chemistry, Faculty of Chemistry and Geosciences, Vilnius University, Naugarduko St. 24, LT-03225 Vilnius, Lithuania

8) Materials Research Center, Y-Carbon Ltd, Kyiv, Ukraine

9) NanoTechnas - Center of Nanotechnology and Materials Science, Institute of Chemistry, Faculty of Chemistry and Geosciences, Vilnius University, Naugarduko St. 24, LT-03225 Vilnius, Lithuania

10) Department of Nanotechnology, State Research Institute Center for Physical Sciences and Technology, Lithuania

11) MB Sensografa, Kiparisu 29, Vilnius Region, Lithuania

\* simonas.ramanavicius AT ftmc.lt

Pollution control and environmental remediation remain major global challenges. In recent years, MXenes have attracted increasing attention across diverse research fields, including environmental remediation [1]. However, the practical implementation of MXene-based materials in existing technologies or as replacements for conventional materials requires precise control over physicochemical properties and long-term stability [2]. In particular, the surface chemistry of MXenes plays a decisive role in determining their adsorption behavior, catalytic activity, selectivity, and interaction with target pollutants. Functional groups such as -O, -OH, and -F can provide active sites for the capture of heavy metal ions, organic dyes, pharmaceutical residues, and other emerging contaminants. At the same time, a layered structure facilitates rapid ion diffusion and provides an abundant accessible surface area, thereby enhancing removal efficiency and reaction kinetics. These characteristics make MXenes attractive candidates for the development of efficient and selective adsorbents and sensors [3,4].

In this study,  $Ti_3C_2T_x$  MXene was synthesized using a minimally intensive layer delamination (MILD) etching protocol, followed by comprehensive characterization of its key physicochemical properties. After evaluating the structural, morphological, and surface characteristics of the synthesized MXene, the material was used to develop an efficient, reusable adsorbent for environmental remediation. The adsorption kinetics and equilibrium isotherm models were further investigated to elucidate the underlying mechanisms governing the adsorption performance of  $Ti_3C_2T_x$  MXene. In addition, various strategies were examined to improve the stability and shelf-life of MXenes, thereby broadening the practical implementation potential. The results demonstrated that selected modifications can effectively suppress MXene oxidation in aqueous environments while preserving its performance.

---

**KEYWORDS:** MXenes, Wastewater treatment, Stability

---

**ACKNOWLEDGEMENTS:** This project received funding from the Research Council of Lithuania (LMTLT), agreement No S-MIP-24-14.

---

### REFERENCES

- [1] Q. Li, C. Ge, J. Ma, S. Gu, H. Yang, Y. Xiong, H. Zhou, H. Du, H. Zhu, Q. Wang, “MXenes-based adsorbents for environmental remediation”, *Separation and Purification Technology*, 342, 126982 (2024). <https://doi.org/10.1016/j.seppur.2024.126982>
- [2] Sonata Adomaviciute-Grabusove, Anton Popov, Simonas Ramanavicius, Valdas Sablinskas, Kateryna Shevchuk, Oleksiy Gogotsi, Ivan Baginskiy, Yury Gogotsi, Arunas Ramanavicius, “Monitoring  $Ti_3C_2T_x$  MXene Degradation Pathways Using Raman Spectroscopy”, *ACS Nano*, 18(20), 13184-13195 (2024). <https://doi.org/10.1021/acsnano.4c02150>
- [3] A. Popov, V. Lisyte, M. Sapauskiene, S. Ramanavicius, S. Zukauskas, N. Slekiene, I. Baginskiy, V. Zahorodna, O. Gogotsi, Asta Kausaite-Minkstimiene, Almira Ramanaviciene, “MXene-based electrochemical glucose biosensors: Comparative enhancement with Aquivion and Nafion”, *Materials Today Nano*, 32, 2025, 100712 (2025). <https://doi.org/10.1016/j.mtnano.2025.100712>
- [4] I. Navitski, S. Zukauskas, S. Ramanavicius, O. Gogotsi, A. Ramanavicius, “2D MXenes in the design of heavy metal ion sensors (review)”, *Trends in Environmental Analytical Chemistry*, 47, e00270 (2025). <https://doi.org/10.1016/j.teac.2025.e00270>

## Chemical properties of MXenes

V. N. Mochalin<sup>1</sup>

*1) Missouri University of Science and Technology, USA*

\* mochalinv AT mst.edu

A large family of two-dimensional transition metal carbides and nitrides (MXenes) raises interest for many applications due to their high electrical conductivity, mechanical properties, potentially tunable electronic structure, nonlinear optical properties, and the ability to be manufactured in the thin film state. However, their chemistry that is key to development of almost all these applications still remains poorly understood. Our initial attempts to understand MXene reactivity with oxygen and water brought about surprising results and raised profound questions related to reactivity of 2D materials as compared to their bulk analogues. In particular, our well-established classification of carbides is being challenged by these findings. In this presentation we will also discuss our more recent progress in understanding fundamental MXene chemistry and illustrate how this understanding helps to suppress unwanted reactions and prolong stability of these materials. For example, suppressing oxidation and hydrolysis at high pH was demonstrated as an effective way to prolong shelf-life and stability of MXene aqueous colloids. Use of polyphosphate also has been shown to improve chemical stability of MXene aqueous colloids. Other selected examples illustrating connections between understanding MXene chemistry and development of their applications will also be considered.

---

**KEYWORDS:** MXenes, 2D materials, Carbides, Carbonitrides

---

**ACKNOWLEDGEMENTS:** We acknowledge funding support for this research from the National Science Foundation (DMREF-2324156).

---

### REFERENCES

- [1] S. Huang, G. Xiang, V.N. Mochalin, Formation of Hydrocarbons and Carbon Oxides in MXene Reactions With Water Under Varying Oxidative Conditions, *Nanoscale*, 17 (16), 9937-9946 (2025).
- [2] A. Baimenov, C. Daulbayev, S.G. Pouloupoulos, V.N. Mochalin, MXene Filled Hydrogel and Aerogel Composites, *Materials Today*, 78, 79-91 (2024).
- [3] S. Huang, V. Natu, J. Tao, Y. Xia, V.N. Mochalin, M.W. Barsoum, Understanding the Effect of Sodium Polyphosphate on Improving Chemical Stability of Ti<sub>3</sub>C<sub>2</sub>T<sub>z</sub> MXene in Water, *Journal of Materials Chemistry A*, 10 (41), 22016-22024 (2022).
- [4] S. Huang, V.N. Mochalin, Combination of High pH and an Antioxidant Improves Chemical Stability of Two-Dimensional Transition-Metal Carbides and Carbonitrides (MXenes) in Aqueous Colloidal Solutions, *Inorganic Chemistry*, 61 (26), 9877-9887 (2022).
- [5] S. Huang, V.N. Mochalin, Understanding Chemistry of Two-Dimensional Transition Metal Carbides and Carbonitrides (MXenes) with Gas Analysis, *ACS Nano*, 14 (8), 10251-10257 (2020).

## Novel ligand coordinated $Ti_2CT_x$ MXene/Cd-MOF composite for improved hydrogen evolution

B. T. Aksoy<sup>1</sup>\*, B. Çoşut<sup>1</sup>

*1) Gebze Technical University, Turkey*

\* btopaloglu AT gtu.edu.tr

The search for sustainable alternative energy sources is widely regarded as a key approach to addressing the growing energy crisis and environmental challenges. Among the proposed solutions, hydrogen production via photocatalytic water splitting using sunlight stands out as a practical and promising strategy [1]. However, achieving high efficiency requires the development of advanced photocatalysts that can effectively harvest solar energy across a broad range of the visible spectrum, promote efficient charge separation, facilitate electron transport, suppress charge recombination, and maintain long-term stability while remaining environmentally benign. To design a new composite photocatalyst candidate, MXene and MOF materials were combined. MXenes are a recently developed class of two-dimensional materials composed of transition metal carbides, nitrides, or carbonitrides. They are characterized by a large specific surface area, diverse surface functional and terminal groups, exceptionally high electrical conductivity, numerous active sites, intrinsic hydrophilicity, strong mechanical properties, and notable chemical stability [2]. Metal-organic frameworks (MOFs) are hybrid inorganic-organic materials consisting of metal cation centers interconnected by organic ligands, forming extended network structures [3]. MOFs are selected for photocatalytic hydrogen production due to their high surface area, tunable band gap, and controllable, functionalizable crystalline structures.

In this study, a novel Cd-based MOF/ $Ti_2CT_x$  MXene heterostructure was developed as a potential high-performance photocatalyst. A new Cd-MOF was synthesized using a six-armed, phosphorus- and nitrogen-rich hexatopic ligand, and subsequently combined with  $Ti_2CT_x$  through three different methods: ligand-bridged assembly (forming covalent coordination), in situ growth, and physical mixing. Photocatalytic hydrogen evolution experiments conducted under simulated sunlight ( $\lambda > 420$  nm) demonstrated that the ligand-bridged  $Ti_2CT_x$ /Cd-MOF heterostructure achieved the highest activity, with a hydrogen production rate of  $3505 \mu\text{mol h}^{-1} \text{g}^{-1}$  representing a 2.3-fold enhancement over the bare  $Ti_2CT_x$  and Cd-MOF. The superior performance is attributed to the covalent ligand-bridging strategy, which significantly improves interfacial electron transfer and migration, as well as to the synergistic interaction between the MOF and MXene components.

Overall, this work provides a compelling example of designing efficient photocatalytic heterostructures through covalent coordination strategies and contributes valuable insights toward meeting the increasing demand for hydrogen as a clean and sustainable energy carrier.

---

**KEYWORDS:** MXene, MOF, Photocatalyst, Hydrogen energy, Water splitting

---

**ACKNOWLEDGEMENTS:** The authors are highly thankful to the Turkish Academy of Sciences (TUBA), TUBITAK, and BIDEB 2211 for financial and partial support.

---

### REFERENCES

- [1] M. R. Gholipour, C. D. Dinh, F. Béland, T. O. Do, "Nanocomposite heterojunctions as sunlight-driven photocatalysts for hydrogen production from water splitting", *Nanoscale*, 7, 8187-8208 (2015).
- [2] X. Li, X. Yin, M. Han, C. Song, X. Sun, H. Xu, L. Cheng, L. Zhang, "A controllable heterogeneous structure and electromagnetic wave absorption properties of  $Ti_2CT_x$  MXene", *J. Mater. Chem. C*, 5, 7621 (2017).
- [3] S. R. Batten, N. R. Champness, X.-M. Chen, J. Garcia-Martinez, S. Kitagawa, L. Ohrström, "Coordination Polymers, Metal-Organic Frameworks and the Need for Terminology Guidelines", *CrystEngComm*, 14, 3001-3004, (2012).

## Glassy-carbon-assisted electrochemical etching of MAX phases: Control, limitations, and opportunities

K. Siuzdak<sup>1\*</sup>, D. Kouao<sup>1</sup>, J. Gumieniak<sup>2</sup>, A. Kramek<sup>2</sup>, J. Karczewski<sup>3</sup>, K. Grochowska<sup>1</sup>

1) Centre for Plasma and Laser Engineering, the Szewalski Institute of Fluid-Flow Machinery, Polish Academy of Sciences, Fiszerza 14 St., 80-231 Gdańsk, Poland, Poland

2) Rzeszow University of Technology, Poland

3) Gdańsk University of Technology, Poland

\* ksiuzdak AT imp.gda.pl

Electrochemical etching of MAX phases is increasingly considered a promising and safer alternative to conventional MXene synthesis routes relying on concentrated HF [1], yet recent studies clearly indicate that this approach still requires substantial optimization to deliver materials with well-controlled and reproducible structures [2,3]. Reported protocols often struggle with incomplete removal of the A layer, the concurrent formation of carbide-derived carbon, and a narrow processing window between selective etching and destructive oxidation of the  $M_{n+1}X_n$  backbone.

In our setup, a glassy carbon crucible acts as the working electrode, a glassy carbon rod serves as the counter electrode, and an Ag/AgCl/0.1 M KCl electrode is used as the reference. The MAX phase is electrochemically etched in an aqueous electrolyte containing tetramethylammonium tetrafluoroborate dissolved in sulfuric or phosphoric acid, which provides a fluorine-containing anion without the use of bulk HF solutions and allows tuning of the proton activity and ionic strength. The process is performed for 48 h at a constant potential of 2 V versus Ag/AgCl, enabling a gradual weakening and removal of the A-layer while maintaining a well-defined electrochemical driving force. This controlled potential regime is intended to minimize uncontrolled corrosion and over-oxidation that frequently accompany purely galvanostatic or two-electrode configurations.

Scanning electron microscopy reveals the formation of layered, accordion-like morphologies characteristic of MXenes, with expanded interparticle gaps indicative of successful interlayer opening. Raman spectra exhibit bands typical of MXene phases, confirming preservation of the  $M_{(n+1)}X_n$  framework and substantial removal of the A element from the parent MAX phase. At the same time, the extended etching time and relatively high anodic potential promote defect generation and local over-oxidation, which we highlight as an intrinsic limitation of the current protocol and a key target for further optimization.

By juxtaposing our results with the existing electrochemical etching literature, we discuss the main advantages (HF-free operation, potential tunability, access to diverse surface terminations) and drawbacks (possible defect-rich products, competing side reactions, sensitivity to electrolyte composition) of this route toward “greener” MXene synthesis. We argue that a carefully designed three-electrode configuration with a glassy-carbon working vessel provides a convenient platform to systematically map the etching window in terms of potential, time, and electrolyte chemistry, and thus to rationally tailor electrochemical protocols that can realistically compete with HF-based methods in terms of safety and MXene quality.

---

**KEYWORDS:** MXene, Electrochemical etching, Glassy carbon, Chronoamperometry, HF-free

---

**ACKNOWLEDGEMENTS:** This work was financially supported by the National Science Centre (Poland) via M-ERA.NET grant no.: 2024/06/Y/ST11/00223.

---

### REFERENCES

- [1] C.E. Shuck, A. Sarycheva, M. Anayee, A. Levitt, Y. Zhu, S. Uzun, V. Balitskiy, V. Zahorodna, O. Gogotsi, Y. Gogotsi, “Scalable Synthesis of  $Ti_3C_2Tx$  MXene”, *Adv. Eng. Mater.* 22, 1901241 (2020)
- [2] D.-S. Kouao, K. Siuzdak, “Electrochemical synthesis of MXenes: a promising leap beyond hydrothermal MAX phase etching”, *2D Materials* 13, 012003 (2026)
- [3] M. Ostermann, M. Piljević, E. Akbari, P. Patil, V. Zahorodna, I. Baginskiy, O. Gogotsi, C. Gachot, M. Rodríguez Ripoll, M. Valtiner, P. Bilotto, “Pulsed Electrochemical Exfoliation for an HF-Free Sustainable MXene Synthesis”, *Small* 21, 2500807 (2025)

## Effect of different surface terminations and single atom catalyst on MXene's reactivity for water dissociation: A density functional theory investigation

T. Kalsoom<sup>1</sup>\*, M. Kolos<sup>1</sup>, F. Karlický<sup>2</sup>

1) Department of Physics, Faculty of Science, University of Ostrava, Czech Republic

2) University of Ostrava, Czech Republic

\* Talha.Kalsoom AT osu.cz

Transition metal carbides (MXenes), a class of two-dimensional (2D) materials, are a promising candidate for catalytic applications due to their remarkable surface reactivity. Numerous theoretical and experimental studies clearly illustrated that surface termination and its variation have a great influence on the catalytic performance of MXenes. Motivated by recent advances in MXene-based catalysis by Kolos et al. [1] and Gouveia et al.[2], we are studying the water dissociation reaction on a set of MXene ( $M_2CT_2$ , where M represents transition metals such as Sc, Ti, V, and Cr, while T refers to functional group O and F) by performing density functional theory (DFT) calculations. Our primary goal is to investigate the impact of different surface termination groups, both in their pristine and defective (vacancy) forms, on MXene's reactivity as a catalyst for water dissociation. Furthermore, one of the effective methods that increases catalytic activity is single-atom catalysis (SAC). SAC maximizes the atomic efficiency of metals and offers a different way to adjust the activity and selectivity of catalytic reactions by dispersing or coordinating a single atom with surface atoms of appropriate support [3]. In this context, we additionally investigate the impact of Pd as a SAC anchored on specific MXene surfaces to analyze how its presence changes the reaction geometry of the water molecule and dissociation energy on the MXene surface. We aim that this work will provide valuable insight for improving MXenes in catalytic processes.

---

**KEYWORDS:** MXenes, Water gas shift reaction, Density functional theory, Catalysis

---

**ACKNOWLEDGEMENTS:** This work was supported by the University of Ostrava (SGS01/PrF/2025) and the European Union under the LERCO project (number CZ.10.03.01/00/22\_003/0000003) via the Operational Programme Just Transition. The calculations were performed at IT4Innovations National Supercomputing Center (e-INFRA CZ, ID 90254).

---

### REFERENCES

- [1] M. Kolos and F. Karlický, “Computational screening of MXene-based catalysts for chlorinated hydrocarbons removal”, *J. Phys. Mater.*, 8, 035001 (2025).
- [2] J. D. Gouveia, A. Morales-Garcia, F. Vines, F. Illas, and JRB Gomes, “MXene as promising catalysts for water dissociation”, *Appl. Catal. B: Environ.*, 260, 118191 (2020).
- [3] H. Oschinski, A. Morales-Garcia, and F. Illas, “Interaction of First Row Transition Metals with  $M_2C$  ( $M = Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, \text{ and } W$ ) MXenes: A Quest for Single-Atom Catalysts”, *J. Phys. Chem. C*, 125, 2477-2484 (2021).

## High-throughput study of mixed-termination effects in MXenes: From electronic structure to transport

M. Novotny<sup>1\*</sup>, F. Karlicky<sup>2</sup>

1) Department of Physics, Faculty of Science, University of Ostrava, Czech Republic

2) University of Ostrava, Czech Republic

\* michal.novotny AT osu.cz

High-performance computing strongly accelerated computational screening in the prediction of nanomaterial properties. Two-dimensional materials represent such a platform for tuning material properties through atomic-scale modifications, with MXenes representing a prominent class due to their metallic conductivity, hydrophilicity, and chemically active surfaces.[1] Their properties are strongly influenced by surface terminations, which are inherently present and difficult to control experimentally. The most common terminal groups (F, O, OH, Cl) have a significant impact on the stability, electronic structure, optical properties, and transport properties of  $M_2CT_2$  (M = Sc, Ti, V, Cr) MXenes.[2,3] While prior studies have focused on idealized, uniformly terminated systems, experimental samples exhibit mixed surface compositions, leading to large variations in reported properties, particularly electrical conductivity. A systematic understanding of how mixed terminations determine intrinsic material behavior is still lacking.[4,5]

We have addressed these issues by quantifying the effects of mixed surface terminations on the electronic structure and transport properties of  $M_2CT_2$  MXenes. We show that terminal groups on opposite sides of the MXene are effectively independent, and that the properties of the material are governed primarily by the overall surface composition rather than by specific surface patterns. To address the large configurational space of mixed terminations, we employ a high-throughput computational approach combining efficient parallelization strategies with a self-developed code for automated generation of structural variations. This enables systematic sampling of a wide range of compositions and configurations while maintaining computational feasibility. The observed independence of surface terminations further reduces the effective configurational complexity, as variations in surface arrangement have a negligible impact on cohesion energy and band structure. At the same time, semiconducting MXenes exhibit extreme sensitivity to conduction-inducing terminations, with concentrations as low as ~1% sufficient to close the band gap, explaining the difficulty of their experimental realization. Transport calculations yield conductivities on the order of 300 kS/m and show nearly constant carrier relaxation times, enabling simplified treatment of mixed systems. These results establish a direct link between surface composition and measurable properties in MXenes.

---

**KEYWORDS:** MXenes, Ab-initio, Surface functionalization, Mixed termination, Transport properties

---

**ACKNOWLEDGEMENTS:** This work has been produced with the financial support of the European Union under the LERCO project (number CZ.10.03.01/0022\_003/0000003) via the Operational Programme Just Transition and the University of Ostrava (number SGS01/PrF/2025). The computations were performed at IT4Innovations National Supercomputing Center through the e-INFRA CZ (ID:90254).

---

### REFERENCES

- [1] T.L. Tan, H.M. Jin, M.B. Sullivan, B. Anasori, Y. Gogotsi: High-Throughput Survey of Ordering Configurations in MXene Alloys Across Compositions and Temperatures. *ACS Nano*, 11, 4407 (2017).
- [2] Y. Gogotsi, Q. Huang: MXenes: Two-Dimensional Building Blocks for Future Materials and Devices. *ACS Nano*, 15, 5775 (2021).
- [3] J. Kalmár, F. Karlický: Strain-induced changes of electronic and optical properties of Zr-based MXenes. *J. Appl. Phys.*, 135, 244302 (2024).
- [4] M. Novotný, K. Tkáčová, F. Karlický: The effect of mixed termination composition in Sc, Ti, and V-based MXenes. *Phys. Chem. Chem. Phys.*, 26, 25514 (2024).
- [5] B. Vénosová, F. Karlický: MXene's Surface Functionalization Patterns and Their Impacts on Magnetism. *Phys. Chem. Chem. Phys.*, 26(26), 18500 (2024).

Posters

T2-08

POSTER

**Reproducible colloidal stability of Au@MXene nanohybrids via ionic environment modulation for biosensing applications**

M. Fatima<sup>1</sup>\*, Z. Babar<sup>2</sup>, B. Della Ventura<sup>2</sup>, R. Velotta<sup>2</sup>, V. Iannotti<sup>2</sup>

1) University of Naples Federico II, Pakistan

2) University of Naples Federico II, Italy

\* mariam.fatima AT unina.it

2D nanomaterials have attracted significant attention due to their unique physicochemical properties and potential in advanced sensing technologies. Among these, MXenes are particularly promising owing to their high surface area, excellent electrical conductivity, and tunable surface chemistry. However, their colloidal stability—especially after surface functionalization—remains a critical limitation for practical applications. MXene-based nanohybrids, such as Au-decorated  $Ti_3C_2TX$  MXenes, have been widely explored to enhance functionality in biosensing platforms. In our system, gold (Au) nanoparticles are formed in situ on MXene flakes via self-assembly. However, nanoparticle incorporation and surface modification processes can alter surface charge characteristics, reduce dispersion stability and limit effective utilization. This issue is further compounded by the lack of systematic reproducibility studies in MXene-based systems. Here, we address the instability of Au@MXene nanohybrids and propose a reproducible strategy to control their colloidal behavior. We demonstrated that controlled ionic environment engineering through citrate addition effectively restores and enhances colloidal stability, achieving a zeta potential of approximately -45 mV. Reproducibility, validated through triplicate experiments, demonstrates consistent particle size and surface charge distributions, addressing a key gap in MXene research. These findings provide a simple and effective approach for stability engineering in MXene-based nanohybrids, facilitating reliable functionalization for biosensing applications. More broadly, this work offers practical insights into the integration of 2D nanomaterials into robust nanodevice platforms.

**KEYWORDS:**  $Ti_3C_2T X$ , MXene nanohybrids, Colloidal stability, Ionic environment control, Gold nanoparticles (AuNPs)

**ACKNOWLEDGEMENTS:** The author acknowledges financial support from the PhD scholarship provided by the University of Naples Federico II, Naples, Italy.

## Synergistic electrochemical performance of $Ti_2VC_2T_x$ MXene and carbon confined metal phosphide heterostructures for advanced energy storage

A. Muhammad<sup>1, 1\*</sup>, A. G. Mahmoud<sup>1</sup>, S. A. Abbas<sup>1</sup>, T. Kennedy<sup>1</sup>

<sup>1</sup> University of Limerick, Ireland

\* Muhammad.adnan AT ul.ie

The rapid growth of portable electronics and electric vehicles has increased the demand for advanced energy storage systems with high power density, large charge storage capacity, and long cycling stability. Two-dimensional transition metal carbides and nitrides, known as MXenes, are promising electrode materials because of their metallic conductivity, hydrophilic surfaces, tunable surface terminations, and surface-controlled charge storage. Among them,  $Ti_2VC_2T_x$ , a  $M_3X_2$ -type MXene, is especially attractive because vanadium incorporation into the titanium carbide lattice improves electronic structure and redox activity. This bimetallic configuration enhances electrochemical reactivity compared to monometallic MXenes. However, pristine MXenes still suffer from nanosheet restacking, which reduces ion accessibility and active surface area, limiting practical capacity.

In this work, we developed a composite electrode by combining  $Ti_2VC_2T_x$  MXene with carbon-confined copper phosphide ( $Cu_3P@C$ ), derived from a copper-based metal-organic framework (MOF) through pyrolysis. A series of  $Ti_2VC_2T_x/Cu_3P@C$  composites with different ratios were systematically studied to identify the best balance between the high conductivity and pseudocapacitive behavior of MXene and the high specific capacity of  $Cu_3P$ . In this structure, MXene sheets form a continuous conductive network for fast electron transport and buffer the volume changes of  $Cu_3P$  during repeated ion insertion and extraction. Meanwhile, the  $Cu_3P@C$  phase provides additional redox-active sites, increasing overall charge storage capacity.

Electrochemical characterization using cyclic voltammetry, galvanostatic charge-discharge, and electrochemical impedance spectroscopy shows that the  $Ti_2VC_2T_x/Cu_3P@C$  heterostructure effectively suppresses MXene restacking and increases the number of electrochemically accessible active sites. Interfacial coupling improves charge transfer kinetics and enables a synergistic storage mechanism combining MXene pseudocapacitance with faradaic redox reactions from  $Cu_3P$ . The presence of multiple redox-active metals (Ti, V, and Cu) also provides richer redox chemistry, improving capacity and expanding the operational potential window.

Overall, this study demonstrates that integrating bimetallic MXenes with carbon-confined metal phosphides is an effective strategy to overcome the limitations of individual electrode materials. By improving interface engineering and ion-accessible surface design,  $Ti_2VC_2T_x$ -based composite electrodes show strong potential for high-rate pseudocapacitive energy storage and next-generation battery technologies.

---

**KEYWORDS:**  $Ti_2VC_2T_x$ , MXene, MOF mediated structures, Copper phosphide, Bimetallic MXenes

---

**ACKNOWLEDGEMENTS:** Adnan Muhammad, Syed Ali Abbas, Abdallah G. Mahmoud, and Tadhg Kennedy\*

---

### REFERENCES

- [1] H. Liu, X. Duan, Z. Wu, H. Luo, X. Wang, C. Huang, Z. Lan, W. Zhou, J. Guo and M. Ismail (2023). "Exfoliation of compact layered  $Ti_2VAIC_2$  MAX to open layered  $Ti_2VC_2$  MXene towards enhancing the hydrogen storage properties of  $MgH_2$ ." *Chemical Engineering Journal* 468: 143688
- [2] M. H. Kong, H. H. Song, J. S. Zhou, *Adv. Energy Mater.* 2018, 8, 1801489. <https://doi.org/10.1002/aenm.201801489>.

## Synergistic enhancement of photocatalytic formaldehyde degradation via CeO<sub>2</sub>/Ti<sub>3</sub>C<sub>2</sub> MXene hybrid

I. Goyal<sup>1\*</sup>, P. Devi<sup>1</sup>, D. Jagadeesan<sup>2</sup>

1) AcSIR, CSIR-CSIO, Chandigarh, India

2) IIT PALAKKAD, India

\* isha.csio21a AT acsir.res.in

Formaldehyde is a major indoor air pollutant posing severe health risks, driving the need for efficient and sustainable removal technologies[1]. In this work novel MXene-based hybrid nanostructure integrating Ti<sub>3</sub>C<sub>2</sub> MXene with CeO<sub>2</sub> was reported for enhanced HCHO degradation under ambient conditions. Ti<sub>3</sub>C<sub>2</sub>-MXene is known for its excellent electronic conductivity and optical properties which act as a promising co-catalyst for the development of efficient photocatalysts[2]. CeO<sub>2</sub> was synthesized using solgel method giving a particle size of less than 5-20 nm and the hybrid was synthesized via chemical mixing[3].

Upon exposure to solar light, CeO<sub>2</sub>/Ti<sub>3</sub>C<sub>2</sub> hybrid demonstrates superior degradation efficiency of nearly 80% as compare to bare CeO<sub>2</sub> (58%) in 240 min which is 1.4 times than bare CeO<sub>2</sub>. The enhanced performance of the CeO<sub>2</sub>/Ti<sub>3</sub>C<sub>2</sub>-MXene hybrid is attributed to the formation of a Schottky junction at the interface and increased surface area of 26.794m<sup>2</sup>/g, which facilitates the transfer of photogenerated electrons promoting efficient charge separation and suppressing electron-hole recombination which leads to faster oxidation of HCHO into CO<sub>2</sub> and H<sub>2</sub>O. This study provides new insights into the design of MXene-based hybrid systems for air purification and underscores their potential in environmental remediation applications

---

**KEYWORDS:** HCHO, CeO<sub>2</sub>, Photocatalysis, Degradation efficiency, Catalytic performance

---

**ACKNOWLEDGEMENTS:** I. Goyal greatly acknowledge AcSIR, CSIR-CSIO, India for providing all the facilities to carry out the research work. The author is thankful to Dr. Pooja Devi, Senior Principal Scientist, CSIR-CSIO, Chandigarh, India and Dr. Dinesh Jagadeesan, Associate Professor, IIT Palakkad, India for their great support.

---

### REFERENCES

- [1] Y. Huang *et al.*, “Removal of Indoor Volatile Organic Compounds via Photocatalytic Oxidation: A Short Review and Prospect,” *Mol.* 2016, Vol. 21, Page 56, vol. 21, no. 1, p. 56, Jan. 2016, doi: 10.3390/MOLECULES21010056.
- [2] Z. Z. J. L. Yujuan Zhang and Peihong Zhang, “Prediction of Ti<sub>3</sub>C<sub>2</sub>O<sub>2</sub> MXene as an effective capturer of formaldehyde,” *Uniw. śląski*, vol. 469, pp. 770-774, 2019, doi: 10.2/JQUERY.MIN.JS.
- [3] A. A. Atran, F. A. Ibrahim, and M. S. Hamdy, “Functionalization and applications of the versatile CeO<sub>2</sub> nanoparticles: A review,” *Inorg. Chem. Commun.*, vol. 163, p. 112359, May 2024, doi: 10.1016/J.INOCHE.2024.112359.

## Reversible sequestration and competitive desorption of resveratrol on $Ti_3C_2T_x$ MXenes

I. Chorna<sup>1\*</sup>, A. Liutyi<sup>2</sup>, S. Kyrylenko<sup>1</sup>, I. Baginskyi<sup>3</sup>, S. Dukhnovskiy<sup>3</sup>, I. Roslyk<sup>3</sup>, V. Zahorodna<sup>3</sup>,  
O. Gogotsi<sup>3</sup>, M. Pogorielov<sup>4, 5</sup>

1) Biomedical Research Center, Academic and Research Medical Institute, Sumy State University, Sumy, Ukraine

2) Sumy State University, Sumy, Ukraine

3) Materials Research Center, Y-Carbon Ltd, Kyiv, Ukraine

4) Institute of Atomic Physics and Spectroscopy, University of Latvia, Latvia

5) Biomedical Research Centre, Medical Institute, Sumy State University, Sumy, Ukraine

\* i.chorna AT med.sumdu.edu.ua

The key concept in the design of 2D nanomaterials for drug and bioactive compound delivery is to achieve a balance between payload retention and local release to minimise premature elimination and systemic toxicity.  $Ti_3C_2T_x$  MXenes are promising nanocarriers, but their dynamic interactions with hydrophobic payloads and systemic transport proteins require further study. This work aims to elucidate a time-dependent, competitive desorption mechanism in a ternary system consisting of  $Ti_3C_2T_x$  MXenes, the hydrophobic polyphenol trans-resveratrol (3,5,4'-trihydroxystilbene, Res), and bovine serum albumin (BSA).

UV-visible, steady-state, and synchronous fluorescence spectroscopy studies showed formation of a complex in binary systems ( $Ti_3C_2T_x$ -BSA,  $Ti_3C_2T_x$ -Res, BSA-Res) and in a ternary system, consisting of BSA introduced to  $Ti_3C_2T_x$  MXenes pre-incubated for 1 h with Res. Dual-wavelength fluorescence spectroscopy at excitations 278 nm and 300 nm was employed to monitor emission states of BSA and Res, respectively, during 1-hour and 24-hour incubations at physiological temperature (37°C). Short-term incubation indicated that  $Ti_3C_2T_x$  MXenes rapidly adsorbed Res and acted as a “kinetic sponge”, holding a significant portion of the polyphenol, thereby decreasing its initial release and its interaction with BSA.

In contrast, long-term incubation resulted in a complete reversal of this effect: the 24-hour ternary system exhibited synergistic quenching (Stern-Volmer quenching ratios  $F_0/F=4.10$ , compared to the 3.27 in binary BSA-Res system) and an expansion in binding stoichiometry (number of binding sites  $n=1.32$  compared to the 0.75 in binary BSA-Res system). Following 24 h of thermodynamic equilibration,  $Ti_3C_2T_x$  MXenes released more than 90% of Res into BSA. The ternary  $Ti_3C_2T_x$ -Res-BSA complex exhibited decreased fluorescence intensity with increasing Res concentration (1.56-12.5 µg/ml) and a red shift (bathochromic) in wavelength, suggesting changes in BSA - polar environment around tryptophan residues. These results demonstrate that  $Ti_3C_2T_x$  MXenes induced conformational unfolding of BSA, exposing previously inaccessible hydrophobic pockets and increasing its binding capacity for Res.

Thus,  $Ti_3C_2T_x$  MXenes may serve as affinity-responsive, time-release nanocarriers that protect hydrophobic small molecules during initial circulation and enhance their target bioavailability.

**KEYWORDS:**  $Ti_3C_2T_x$ , Nanocarriers, Fluorescence quenching, Bovine serum albumin, Resveratrol

**ACKNOWLEDGEMENTS:** Supported by Air Force Office of Scientific Research via EOARD project P809, NAS funded IMPRESS-U project #7128, projects #0126U000874 and #0124U000637 of the Ministry of Education and Science of Ukraine, ERASMUS-JMO-2023-MODULE project #101127618 MedFood.

# Track 3

Quantum Materials, Devices, and Phenomena

## Exciton-stimulated emission of a SnO thin film on a Sn plate formed by Nd:YAG laser oxidation

A. Medvids<sup>1</sup>\*

1) Riga Technical University, Latvia

\* medvids AT latnet.lv

Tin oxide (SnO) crystal is an indirect band-gap semiconductor with  $E_g=0.9$  eV, but intensive luminescence takes place at direct transition with energy  $E_g = 2.5-3.6$  eV, and 98 meV exciton binding energy at room temperature. Therefore, it has been successfully used in optoelectronics, energy storage devices, and sensors [1]. However, there is no significant research or clear indication in the literature suggesting that SnO thin films are capable of or have been used for lasing. Therefore, the aim of our investigation is to find the conditions under which SnO thin film can be used for lasing. A plate of Sn with 99.5% purity was irradiated with pulses of the Nd: YAG laser at a wavelength of  $\lambda=1064$  nm, and the frequency of repetition of laser pulses was 10Hz. The irradiation of 5 lines with intensities  $I_1=6$  GW/cm<sup>2</sup>,  $I_2=5.5$ GW/cm<sup>2</sup>,  $I_3=3$  GW/cm<sup>2</sup>,  $I_4=3.6$  GW/cm<sup>2</sup> and  $I_5_{min}= 2$  GW/cm<sup>2</sup> were used in experiments. Photoluminescence (PL) spectra and relaxation spectra were measured using femtosecond laser excitation ( $\tau_p = 180$  fs) at  $\lambda = 266$  nm, with a regulated excitation pulse fluence in the 8  $\mu$ J/cm<sup>2</sup>-1.7 mJ/cm<sup>2</sup> range. The PL spectra were measured with 20 ps temporal resolution. The diameter of the laser beam spot was 125  $\mu$ . The structural properties and phase composition of the films were studied using a Raman spectrometer in backscattering geometry at room temperature [2]. The phonon excitation was induced with an Ar<sup>+</sup>- laser ( $\lambda_{ex} = 514.5$  nm). XRD structural characterization was performed on a Rigaku SmartLab diffractometer (Japan) equipped with a scintillation detector SC-70. An optical microscope with UV illumination of the sample was used to visualize invisible (transparent) SnO thin films. It was found that all irradiated zones exhibit a typical SnO crystal PL spectrum with two bands: an excitonic band at a maximum wavelength of 375 nm and a defect-related band at 450 nm. The relation intensities of these bands  $I_{ex}/I_{df}$  determine the quality of the crystal [3] and the highest is 100 for 5 zone. It means that the best crystallinity of the SnO thin film is obtained at Nd: YAG laser irradiation intensity of 2 GW/cm<sup>2</sup> and is characterized by exciton-stimulated emission at  $\lambda=375$  nm. The lasing emission threshold is  $I_{th} = 0.8$  mJ/cm<sup>2</sup> when excited by a femtosecond laser at  $\lambda = 266$  nm. It was found that the best crystallinity of the SnO thin film is obtained at Nd: YAG laser irradiation intensity of 6 GW/cm<sup>2</sup> and is characterized by exciton-stimulated emission at  $\lambda=375$  nm. The lasing emission threshold is  $I_{thr} = 0.8$  mJ/cm<sup>2</sup> when excited by a femtosecond laser at  $\lambda = 266$  nm.

---

**KEYWORDS:** Nd, YAG laser, Sn laser, Laser oxidation, Visualization

---

### REFERENCES

- [1] O. Mounkachi, E. Salmani, M. Lakhali, H. Ez-Zahraouy, M. Hamedoun, and A. Benyoussef, *Solar Energy Materials and Solar Cells*, 148, 34 (2016).
- [2] B. Eifert, M. Becker, Christian T.Reind, Peter Klar, *Phys Rev Mater.*, 1(1):014602 (2017).
- [3] J. Kaupužs, A. Medvids, P. Onufrijevs, H. Mimura, *Optics & Laser Technology*, 111, 121 (2019).

## Explore flat-bands with artificial atomic lattices

H. Ding<sup>1</sup>\*

*1) Department of Physics, Nanjing University, 210093 Nanjing, China*

\* hfding AT nju.edu.cn

Flat-bands yield electrons in the band with vanishing group velocity and divergent effective mass, promoting strong correlation physics. Previous investigations only found a rather limited number (~10) of 2D flat-band lattices with the number of the sites in an unit cell less than 10. In addition, the flat bands of many well-known lattices, such as Lieb and kagome lattices are obtained with the nearest neighbor (NN) hopping only. The adding of the higher order NN hopping, however, strongly influences the flatness of the band and the originally predicted flat-band is no longer flat.

In this talk, I will present our recent studies of flat-bands with artificial atomic lattices. In Fe adatom on Ag(111), we found a surface state assisted long range hopping between adatoms, where the hopping shows an inverse square dependence with their separation rather than the commonly thought exponential one [1]. With this system, we demonstrate a band compression effect with can effectively compress the bandwidth of a particular band and convert it to a flat band [2]. Further, we show a general method for realizing flat bands based on mathematical optimization and symmetry analysis. The method allows us to find over 1000 flat-band lattices, implying flat-band structures are far more abundant than previously thought [3]. Moreover, in a joint tight-binding and experimental efforts, we demonstrate a convenient approach to tune the Flat-band energy in an almost continuous manner [4]. These findings suggest that the artificial atomic structures can serve as an interesting playground to explore the rich flat-band physics.

---

**KEYWORDS:** Flat-bands, Artificial atomic lattices, Scanning tunneling microscopy, Atomic manipulation

---

**ACKNOWLEDGEMENTS:** These projects are supported by MOST and NSFC.

---

### REFERENCES

- [1] X. Li *et al.*, Chin. Phys. Lett., 39, 057301, (2022)
- [2] R. Yan *et al.*, Phys. Rev. B, 108, 075153, (2023)
- [3] H. Li *et al.*, Phys. Rev. Lett., 134, 076402, (2025)
- [4] H. Li *et al.*, submittal, (2026)

## Toward quantum circuits based on topological insulators

D. Carroll<sup>1</sup>\*

*1) Department of Physics, Wake Forest University, USA*

\* carrold1 AT wfu.edu

The topological edge states of 2D topological insulators are known to be robust against any perturbation that respects time reversal symmetry. Such topological protection allows for nearly dissipationless dynamical states suggesting a potential route to long dephasing times and higher energy scales in quantum systems. In this work we explore a 2D materials system which combines the band topology of chalcogenides ( $\text{Sb}_2\text{Te}_3$ ) with the unique quantum geometry of a twinned crystalline spiral manifold. We show that the edge-symmetries are reflected in the dislocations that allow for the twinned, mirrored crystal structure. Using a combination of electron energy loss spectroscopy, magnetic force microscopy and dc magneto-transport, we identify bandgap states with specific excitation transitions of  $\sim 0.18$  eV. This suggests that the symmetry considerations of such spiral crystals, modifies the bandgap topological edge band in such a way to restrict available states to just two, well separated energy levels. With such crystals placed within the pickup capacitor of a resonator circuit, that circuit has two distinct resonance frequencies. We show that the measurement of the resonance frequency of such circuits is generally probabilistic and that the probability of a given frequency can be altered by the introduction of voltage pulses into the circuit. This work opens important possibilities in the use of 2D chalcogenides in novel circuit geometries.

---

**KEYWORDS:** Topological materials, Quantum geometry, Qubits

---

**ACKNOWLEDGEMENTS:** this work was funded by QUOHERENT INC.

---

### REFERENCES

- [1] C.L. Kane, E.J.Z. Mele, 2 Topological Order and the Quantum Spin Hall Effect. PRL 95, (2005).
- [2] S. Murakami, Quantum Spin Hall Effect and Enhanced Magnetic Response by Spin-Orbit Coupling. Phys. Rev. Lett. 97, 236805 (2006).
- [3] H. Zhang, *et al.* Topological insulators in  $\text{Bi}_2\text{Se}_3$ ,  $\text{Bi}_2\text{Te}_3$  and  $\text{Sb}_2\text{Te}_3$  with a single Dirac cone on the surface. Nature Phys 5, 438-442 (2009).
- [4] C. Dun, *et al.*  $\text{Bi}_2\text{Te}_3$  Plates with Single Nanopore: The Formation of Surface Defects and Self-Repair Growth. Chem. Mater. 30, 1965-1970 (2018).
- [5] R. Link, G. Marcus, D. Carroll, Solvothermal growth of moiré superlattices in antimony telluride spiral-type nanoplates. Frontiers in Materials 9, (2022).

## From charge to emerging quantum states: Rare-earth complexes on surfaces

S. W. Hla<sup>1</sup>\*

*1) Ohio University, USA*

\* hla AT ohio.edu

Complexes containing rare-earth ions attract great attention for their technological applications, ranging from spintronic devices to quantum information science. In the rare-earth-based molecules, the interaction between the metal atom and local electronic states plays a vital role in determining their properties. This can be exploited by engineering molecular ligands to tailor them for desired applications. These molecular ligands not only protect the rare-earth atoms from the surrounding environment but also influence their electronic and magnetic properties [1,2]. We have designed a variety of rare-earth (Eu, Tb, Er, La, and Lu) based molecular complexes and studied their self-assemblies on noble metal surfaces using low-temperature scanning tunneling microscopy (STM) and tunneling spectroscopy combined with synchrotron X-ray experiments. We are able to form molecular complexes that retain the charge state of rare-earth ions on metallic surfaces, opening their potential applications in a solid-state environment. In some rare-earth clusters, the self-assembled structures are formed by electrostatic and dispersive interactions [3]. Many of these complex assemblies are chiral and exhibit exotic properties on metallic surfaces, including quantum superposition and internal Stark effects. Internal polarizability induced by counterions is also investigated, not only on individual complexes on metallic surfaces, but also on artificially assembled complex structures using STM molecular manipulation schemes [4].

---

**KEYWORDS:** Rare-Earth, STM, Synchrotron X-rays, Atomic manipulation, Metal surfaces

---

**ACKNOWLEDGEMENTS:** We gratefully acknowledge financial support from the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Materials Science and Engineering Division. Work performed at the Center for Nanoscale Materials and Advanced Photon Source, both U.S. Department of Energy Office of Science User Facilities, was supported by the U.S. DOE, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357. We acknowledge the computing resources provided on Bebop, a high-performance computing cluster operated by the Laboratory Computing Resource Center at Argonne National Laboratory.

---

### REFERENCES

- [1] T.M. Ajayi, N. Shirato, T. Rojas, S. Wiegold, X. Cheng, K. Z. Latt, D. J. Trainer, N. K. Dandu, Y. Li, S. Premarathna, S. Sarkar, D. Rosenmann, Y. Liu, N. Kyritsakas, S. Wang, E. Masson, V. Rose, X. Li, A. T. Ngo, & S.-W. Hla. *Nature* 618, 69-73 (2023).
- [2] T.M. Ajayi, V. Singh, K.Z. Latt, S. Sarkar, X. Cheng, S. Premarathna, N.K. Dandu, S. Wang, F. Movahedifar, S. Wiegold, N. Shirato, V. Rose, L.A. Curtiss, A.T. Ngo, E. Masson, and S.-W. Hla. *Nat. Commun.* 13, 6305 (2022).
- [3] D. Trainer, K. Z. Latt, X. Cheng, N. K. Dandu, L. A. Curtiss, S. E. Ulloa, A. T. Ngo, E. Masson, & S. W. Hla. *ACS Nano* 19, 15272-15280 (2025).
- [4] D. Trainer, A. T. Lee, S. Sarkar, V. Singh, X. Cheng, N. K. Dandu, K. Z. Latt, S. Wang, T. M. Ajayi, S. Premarathna, D. Facemyer, L. A. Curtiss, S. E. Ulloa, A. T. Ngo, E. Masson, & S. W. Hla. *Adv. Sci.* 2308813 (2024).

## Quantum energy teleportation and effective thermodynamics

H. Matsueda<sup>1</sup>\*

*1) Graduate School of Engineering, Tohoku University, Japan*

\* hiroaki.matsueda.c8 AT tohoku.ac.jp

Whether quantum informational resources can be converted into energy is a fundamental physical question, and it is also a question closely connected to the development of quantum technology. Quantum energy teleportation (QET) is a protocol in which energy is extracted at a distant location by performing projective measurement, classical communication, and feedback operation on the ground state of a quantum many-body system with entanglement. Since thermodynamics involving measurement and operation is incomplete, the information-thermodynamic and quantum-thermodynamic understanding of QET is still insufficient. This study clarifies the first and second laws of effective thermodynamics. The entire system is a quantum system at zero temperature, but the subsystem from which energy is extracted experiences effective temperature effects due to interactions with other subsystems. First, in relation to the first law of thermodynamics, the ways in which heat and work are defined were clarified. Next, in relation to the second law of thermodynamics, it was proven that the upper bound of locally extractable energy can be transformed into the same form as the famous Sagawa-Ueda inequality. To effectively advance the above research, we employed a Kitaev quantum liquid-like one-dimensional spin model. This model has interactions that differ for each bond, which allows us to clearly describe how the non-commutativity of feedback operations and interactions affects energy control. Our results are based on specific models and are by no means general, but it can be said that this is a valuable study in the sense that it provides mathematically rigorous results on issues that many researchers in this field are interested in, such as the definitions of work and heat in quantum thermodynamics and the second law of information thermodynamics.

---

**KEYWORDS:** Quantum energy teleportation, Entanglement, LOCC, Information thermodynamics, Kitaev quantum spin liquid

---

**ACKNOWLEDGEMENTS:** This work is supported by JSPS KAKENHI Grants No. JP24K06878, No. JP24K00563, No. JP2402948, and No. JP23K22492, and CSIS in Tohoku University.

---

### REFERENCES

- [1] H. Matsueda, Y. Masaki, K. Itoh, A. Ono, and J. Nasu, "Nonlocal correlations in quantum energy teleportation: Perspectives from their Majorana representations and information thermodynamics", *Phys. Rev. Res.* 7, 033137 (2025)
- [2] K. Itoh, Y. Masaki, and H. Matsueda, "Upper bound on locally extractable energy from entangled pure state under feedback control", *Phys. Rev. E* 113, 024108 (2026)

## Kondo screening and entanglement of spin states on graphene nanoribbon

A. Hassanien<sup>1</sup>\*

*1) Jozef Stefan Institute, Slovenia*

\* Abdou.Hassanien AT ijs.si

Exploring the spatial dependence of mediated exchange interactions is very useful to understand the mechanism of magnetic ordering and entanglement of spin states. The confined structure and low spin-decoherence channel of 7-armchair graphene nanoribbon (7-AGNR) offer a suitable platform to partially isolate the effect of substrate and visualize the competition between exchange interactions and Kondo screening. Herein, we use scanning tunneling methods to map the spatial dependence of local density of states between two unpassivated sites across the terminus of 7-AGNR. A well-pronounced pair of delocalized Kondo resonances were observed which gradually decay away from the scattering centers but still visible at any point along the line profile. This ubiquitous presence of Kondo effect indicates mediated exchange interactions that may lead to magnetic ordering or exotic coupling between spin states. Although thermal decoherence weakens the signal intensity, temperature dependence shows that the interaction effects remain detectable at relatively high temperature of 15K. As the coupling strength of the two delocalized moments could be tuned by electric field, this system offers a great potential for applications in devices employing quantum information processing.

---

**KEYWORDS:** Graphene nanoribbons, Spin states, Exchange interactions, Scanning tunneling microscopy

---

### REFERENCES

- [1] Stefan Šćepanović, Amina Kimouche, Jovan Mirković, Gehad Sadiq, Tillmann Klamroth and Abdou Hassanien. Delocalized spin states at zigzag termini of armchair graphene nanoribbon. *Sci Rep* 14, 11641 (2024).
- [2] A. Hassanien. Robust Contact by Direct Formation of C-Au Bond in Suspended Armchair Graphene Nanoribbon. *Phys. Status Solidi RRL*, 18: 2470030 (2024).
- [3] Stefan Šćepanović, Diego López-Alcalá, José J Baldoví, Alexander Vahl, Abdou Hassanien. *Phys. Status Solidi RRL*, 19:e2500203 (2025).

T3-07

INVITED

## Mesoscopic Josephson array with permutation symmetry: A lattice-gauge building block

M. Yu<sup>1</sup>, H. Bi<sup>2</sup>, D. Green<sup>3</sup>, C. Chamon<sup>2</sup>, N. Mason<sup>1</sup>, A. Higginbotham<sup>1</sup> \*

1) *University of Chicago, USA*

2) *Purdue University, USA*

3) *Boston University, Ising Ventures, USA*

\* ahigginbotham AT uchicago.edu

I will describe a new category of superconducting qubit where the Josephson junction is replaced by a mesoscopic Josephson array. The qubit has a six-fold degenerate ground state. The ground states are related by  $Z_3$  phase rotations, and are eigenstates of a star operator. The qubit is therefore a potential building block of spin liquids. I will report the design and experimental spectroscopy of the simplest example of this qubit.

---

**KEYWORDS:** Mesoscopic Josephson arrays, Superconducting qubits, Lattice-gauge models, Quantum information

---

**ACKNOWLEDGEMENTS:** DOE DE-SC0026189, NOMIS Foundation

## Investigation of spin systems and evolving quantum states using quantum programming

K. Gnatenko<sup>1</sup> \*

*1) Ivan Franko National University of Lviv, Ukraine*

\* khrystyna.gnatenko AT gmail.com

Evolving quantum states of spin systems that can be described by weighted graphs  $G(V,E)$  are considered [1]. The study focuses on the geometrical properties of these states. In particular, the velocity, curvature, and torsion are obtained analytically for the general case of quantum states corresponding to graphs of arbitrary structure. We establish relationships between these quantum characteristics and the classical properties of the corresponding graphs [1]. We show that the velocity of quantum evolution is related to the sum of the weighted vertex degrees in a graph obtained by squaring the edge weights of  $G(V,E)$ . The curvature depends on the sums of products of edge weights corresponding to square subgraphs in the graph. The torsion depends on sums of products of edge weights forming triangular subgraphs in the graph. The geometric characteristics of quantum graph states are evaluated using quantum programming on IBM quantum computers for the particular case of spin systems [1].

Quantum entanglement plays a crucial role in quantum information science and is one of the key resources for quantum computing and quantum programming. The entanglement distance for evolving quantum states of spin systems described by the XXZ model is investigated both analytically and by means of quantum-computing methods [2]. In addition, the speed of evolution of a two-spin system governed by the XXZ model is examined. The quantum-computational results are consistent with the theoretical predictions.

Multi-qubit quantum states associated with bi- and tripartite graphs are also considered. We establish a direct connection between the entanglement properties and the degrees of the graph vertices [3,4]. Furthermore, relationships between quantum correlators, the numbers of odd- and even-degree vertices, and the numbers of closed cycles of order four are determined. Based on these findings, quantum protocols are developed for evaluating the properties of bi- and tripartite graphs [3,4].

---

**KEYWORDS:** Spin systems, Quantum states, Quantum programming

---

**ACKNOWLEDGEMENTS:** This work was supported by Project 2025.07/0326 (No. 0126U002943) from National Research Foundation of Ukraine.

---

### REFERENCES

- [1] Kh. P. Gnatenko “Relation of curvature and torsion of weighted graph states with graph properties and its studies on a quantum computer”, *Eur. Phys. J. Plus* 140(3), 241 (2025).
- [2] M. P. Tonne, and Kh. P. Gnatenko “Quantifying the properties of evolutionary quantum states of the XXZ spin model using quantum computing”, *arXiv:2601.10650* (2026).
- [3] Kh. P. Gnatenko “Studies of properties of bipartite graphs with quantum programming”, *Phys. Lett. A* 566, 131191 (2026).
- [4] Kh. P. Gnatenko “Entanglement of multi-qubit quantum graph states and studies structural properties of tripartite graphs with quantum programming”, *arXiv:2604.27829* (2026).

## Posters

T3-09

POSTER

### Adaptive SPADE: Superresolving optical imaging for dynamic nanosystems

K. Schlichtholz<sup>1</sup> \*

*1) University of Gdansk, Poland*

\* konrad.schlichtholz AT ug.edu.pl

One of the topics of primary interest in contemporary optics and metrology is superresolution techniques, which allow for efficient resolution below the Rayleigh limit. Recent advances in quantum metrology demonstrate that spatial mode demultiplexing (SPADE) followed by photon counting is quantum optimal for estimating the separation between two weak incoherent sources [1]. While this has drawn significant attention to the technique, the main research focus has concentrated on astronomical applications [2], despite early suggestions for its use in microscopy [1]. In our work [3], we explore the potential application of this method to resolving sources in solutions where Brownian motion presents a major challenge to imaging, an effect that is unavoidable in biological systems. Through Fisher information analysis, we show that utilizing an adaptive scheme with realignments on a properly tuned timescale allows for preserving the optimal quantum scaling of error with separation. We also discuss the realignment time that enables near-optimal scaling while being more feasible for experimental realization. Our findings could help adapt SPADE to examining synthesized nanostructures, e.g., by counting the number of attached fluorophores, or for tracking molecular systems in living cells.

---

**KEYWORDS:** Superresolution imaging, Spatial mode demultiplexing (SPADE), Quantum metrology, Photon counting

---

**ACKNOWLEDGEMENTS:** Author thank the IRA Programme, project no. FENG.02.01-IP.05-0006/23, financed by the FENG program 2021-2027, Priority FENG.02, Measure FENG.02.01., with the support of the FNP.

---

#### REFERENCES

- [1] M. Tsang, R. Nair, and X.-M. Lu, "Quantum theory of superresolution for two incoherent optical point sources", *Phys. Rev. X* 6, 031033 (2016).
- [2] Z. Huang and C. Lupo, "Quantum hypothesis testing for exoplanet detection", *Phys. Rev. Lett.* 127, 130502 (2021).
- [3] K. Schlichtholz, "Superresolving optical ruler based on spatial mode demultiplexing for systems evolving under Brownian motion", *Physics of Fluids* 37, 027178 (2025)

# Track 4

Electrochemistry of Nanomaterials, and Advanced Energy  
Storage

## Nanoscale metal oxide and metal interlayers for anode-free solid-state lithium metal batteries: Reactivity and lithium plating mechanisms

S. Tepavcevic<sup>1\*</sup>

*1) Argonne National Laboratory, USA*

\* sanja AT anl.gov

Anode-free solid-state lithium-metal batteries offer exceptional energy density, but their cycle life is limited by low Coulombic efficiency, lithium inventory loss from interphase formation, and nonuniform lithium deposition. Here, we investigate a common design strategy using ~ 20 nm artificial layers on Cu current collectors to control lithium nucleation and growth in cells with poly(ethylene oxide)-based solid polymer electrolytes. Ideally, lithium should plate uniformly either beneath or on top of the artificial layer, thereby minimizing continued parasitic reaction with the electrolyte; however, if top-side deposition is nonuniform, dendritic lithium growth can result. We first study metal oxide coatings, Al<sub>2</sub>O<sub>3</sub> and ZnO, which exhibit distinct reaction pathways with lithium. Al<sub>2</sub>O<sub>3</sub> undergoes self-limiting lithiation, reducing SEI-related lithium loss but increasing interfacial resistance and nucleation overpotential, with lithium plating beneath the lithiated coating through defects and ion-conducting phases. In contrast, ZnO fully converts to LiZn and Li<sub>2</sub>O, lowering nucleation overpotential and promoting lithium deposition on top of the converted layer. Motivated by this favorable lithiophilic behavior, we then examine ~ 20 nm alloy-forming metal seed layers of Ag, Pt, and Au on Cu. Among these, Au provides the greatest improvement in Coulombic efficiency, with further gains achieved by restricting cycling to suppress continuous alloying and dealloying. Together, these results show that both conversion-type oxide interlayers and alloy-forming metal seed layers can direct lithium growth, but achieving highly uniform deposition remains critical for preventing dendrite formation and improving reversibility in anode-free solid-state batteries.

---

**KEYWORDS:** Anode-free batteries, Solid-state lithium-metal batteries, Lithium plating, Solid polymer electrolytes, Interphase engineering

## Forcing gold to become good electrocatalyst by tuning its electronic properties

V. Komanicky<sup>1</sup>\*, F. D. Sanij<sup>1</sup>, S. Vorobiov<sup>1</sup>, D. Volavka<sup>2</sup>, R. Bodnarova<sup>1</sup>

1) Department of Condensed Matter Physics, Faculty of Science, P.J. Šafárik University, Park Angelinum 9, 041 54 Košice, Slovakia

2) Centre of Low Temperature Physics, Faculty of Science, Pavol Jozef Šafárik University in Košice, Slovakia

\* vladimir.komanicky AT upjs.sk

Gold is a precious metal regarded as a cornerstone-and sometimes the standard-in investment and finance, primarily due to its scarcity, resilience, and stability. Beyond its financial value, gold's properties such as durability, malleability, and excellent electrical conductivity have enabled numerous industrial applications ranging from aerospace and sustainable energy to computing and healthcare.

However, despite its versatility, gold is a poor catalyst or electrocatalyst. Its high chemical nobility stems from its low reactivity and inability to effectively bind molecules to its surface and facilitate their reactions. Hammer and Nørskov [1] explained this behavior using the d-band theory, which attributes gold's chemical inertness to its fully occupied valence d-band located well below the Fermi level-rendering it unavailable for bonding interactions.

In this work, we demonstrate how the electronic properties of ultrathin gold films can be modified by introducing an underlying layer of a different metal. The proximity of this substrate metal can donate or withdraw electrons from the gold overlayer, thereby enhancing its catalytic activity-particularly toward the oxygen reduction reaction (ORR), a key process in polymer electrolyte fuel cells. Our results show that changes in the electronic structure of gold, measured by X-ray photoelectron spectroscopy (XPS) and Kelvin probe force microscopy (KPFM), correlate strongly with its ORR activity.

---

**KEYWORDS:** Oxygen reduction reaction, Electrocatalysis, Gold

---

**ACKNOWLEDGEMENTS:** This work has been supported by the grants of the Slovak Research and Development Agency under contract APVV-23-0049 and APVV-20-0528.

---

### REFERENCES

[1] B. Hammer, J. Nørskov Why gold is the noblest of all the metals, *Nature* (1995) , 376, 238-240.

## Identifying active sites for alkaline hydrogen evolution on nickel

D. Kozlica<sup>1</sup>, M. Finšgar<sup>2</sup>, M. Huš<sup>1</sup>, M. Martins<sup>1</sup>, O. Vodeb<sup>1</sup>, P. Martins<sup>1</sup>, M. Perčinič<sup>3</sup>, S. Džerovski<sup>3</sup>,  
M. Gaberšček<sup>1</sup>, D. Strmcnik<sup>1\*</sup>

1) National Institute of Chemistry, Ljubljana, Slovenia

2) Faculty of Chemistry and Chemical Engineering, University of Maribor, Slovenia

3) Jožef Stefan Institute, Jamova 39, SI-1001 Ljubljana, Slovenia, Slovenia

\* dusan.strmcnik AT ki.si

Nickel-based materials are among the most widely used non-precious catalysts for alkaline hydrogen evolution, yet the identity of the catalytically relevant active sites on Ni remains debated. The difficulty arises from the dynamic chemistry of Ni surfaces: metallic Ni, oxides, hydroxides and hydride-like species can coexist, evolve with electrochemical history, and influence both intrinsic activity and the number of available sites. As a result, nominally similar Ni catalysts often show widely scattered HER activities.

In this talk, we present our efforts to identify active sites for alkaline HER on Ni through an integrated workflow combining controlled surface preparation, high-precision electrochemistry, electrochemical impedance spectroscopy, electrochemical simulations, surface-sensitive characterization and data-driven ToF-SIMS analysis. We first examine how relevant Ni surface states form in alkaline media. Cyclic voltammetry, potential-hold experiments and simulations of competing oxidation pathways are used to distinguish between direct adsorption, dissolution-precipitation, nucleation-and-growth and place-exchange mechanisms for the initial formation of Ni (hydr)oxide. The results support a place-exchange pathway in which hydroxide adsorption is followed by oxidation to surface oxygen and incorporation beneath an outer hydroxide-rich layer. ToF-SIMS depth profiling reveals the resulting duplex near-surface structure, with NiO located between metallic Ni and Ni(OH)<sub>2</sub>-rich surface regions.

This structural understanding provides the basis for correlating surface chemistry with HER activity. Defined Ni, NiO-, Ni(OH)<sub>2</sub>- and NiH<sub>x</sub>-modified surfaces are used to separate the effects of different surface and subsurface states on HER kinetics. A key methodological challenge is to distinguish changes in intrinsic activity from changes in the number of electrochemically available sites. We therefore extend conventional voltammetric and activity-based analysis with impedance-derived descriptors of interfacial kinetics, active-site availability and surface-state evolution.

Finally, we discuss how ToF-SIMS, combined with multivariate analysis and interpretable machine-learning workflows, can provide chemically resolved information on ultrathin, heterogeneous surface regions. Rather than relying on individual marker ions, our approach treats ToF-SIMS depth profiles as fragment-rich hyperspectral datasets and uses denoising, unsupervised fragment grouping, constrained regression and graph-based source assignment to reconstruct chemically meaningful fragment-ion families.

Together, these results illustrate how active-site identification for alkaline HER on Ni requires linking controlled surface chemistry, electrochemical function, impedance-derived site descriptors and chemically resolved near-surface analysis within a single experimentally constrained framework.

---

**KEYWORDS:** Hydrogen evolution reaction, Nickel electrocatalysts, Active sites, ToF-SIMS, Electrochemical simulations

---

**ACKNOWLEDGEMENTS:** The Slovenian Research and Innovation Agency supported the work (Grant Nos. P2-0118, P2-0152, J7-4636, J7-4638, J2-50058, J7-50227, J1-70039, and I0-0039). The project is co-financed by the Republic of Slovenia, the Ministry of Higher Education, Science and Innovation, and the European Union under the European Regional Development Fund. The research was cofounded under the HyBReED project, supported by the European Union-NextGenerationEU.

---

### REFERENCES

- [1] M. Finšgar, K. A. Varda, D. K. Kozlica, M. Huš, M. Martins, D. Strmcnik. "Combining ToF-SIMS and Multivariate Analysis to Resolve Active Sites on Ni-Based HER Catalysts", *Angew. Chem. Int. Ed.*, 2026, 65, e19929.
- [2] D. Kozlica, M. Finšgar, Martins PFBD, *et al.* "The role of individual nickel surface species in the hydrogen evolution reaction on nickel in alkaline electrolytes." *Research Square*; 2025. DOI: 10.21203/rs.3.rs-7285662/v1.

## Computational studies of electrochemical reactions for energy applications

P. Zapol<sup>1</sup>\*

1) Argonne National Laboratory, Lemont, IL 60439, USA

\* zapol AT anl.gov

Understanding electrochemical processes that interconvert chemical and electrical energy is essential for advances in fuel cells, batteries, and microelectronics. Because these processes are governed by complex interactions among electrode surfaces, adsorbates, and interfacial water, first-principles electronic-structure calculations are central to identifying the origins of electrocatalyst activity and stability. We use density functional theory, together with microkinetic modeling and close integration with experiment, to study nanostructured electrocatalysts for water-splitting and oxygen electrocatalysis. A central challenge in electrochemical hydrogen production is the design of oxygen evolution reaction (OER) catalysts that are both active and stable. To establish a computationally informed understanding of iridium electrochemistry in acid, we investigated Ir(111), Ir(100), and Ir(110) surfaces[1]. Density functional theory and microkinetic adsorption-voltammetry simulations were used to interpret electrochemical measurements and in situ spectroscopy revealing potential-dependent hydrogen, hydroxyl, and oxygen coverages, facet-dependent coadsorption behavior, and the strong influence of lateral interactions and the interfacial water network on adsorption dynamics and reactivity. These results clarify trends in hydrogen oxidation/evolution and oxygen reduction on Ir(hkl) surfaces and refine the atomistic picture needed to design advanced Ir-based materials. We also examine a computational design strategy based on dynamically stable electrocatalysts, in which a PGM-free host couples its structural stability with active species supplied by the electrolyte. First-principles studies of conductive  $M_1O_xH_y$ ,  $Fe-M_1O_xH_y$ , and  $Fe-M_1M_2O_xH_y$  hydr(oxy)oxide nanoclusters ( $M_1 = Ni, Co, Fe$ ;  $M_2 = Mn, Co, Cu$ ) show that OER performance emerges from balancing Fe dissolution and redeposition on a  $MO_xH_y$  host to sustain dynamically stable Fe active sites.[2] Extending this concept to perovskite oxides, our interfacial model describes an electronically conductive  $ABO_3$  core that supports surface evolution into a hydr(oxy)oxide shell, where dynamically stable  $Fe(aq)$  species promote oxygen evolution.[3] Finally, combining first-principles calculations with synthesis and characterization, we investigated how electrolyte Fe and interlayer anions jointly control OER in NiAl layered double hydroxides. While  $CO_3^{2-}$ ,  $Cl^-$ , and  $Br^-$  interlayers give similar activity in Fe-free electrolyte, calculations and experiment show that added Fe enhances performance by tuning interfacial Fe adsorption, with activity following  $LDH-Br > LDH-Cl > LDH-CO_3$  across Fe concentrations.[4]

**KEYWORDS:** Density functional theory, Oxygen evolution reaction, Perovskite

**ACKNOWLEDGEMENTS:** PZ acknowledges support by Laboratory Directed Research and Development (LDRD) funding from Argonne National Laboratory, provided by the Director, Office of Science, of the U.S. Department of Energy under Contract No. DE-AC02-06CH11357. Computational resources provided by the Argonne Laboratory Computing Resource Center are gratefully acknowledged.

### REFERENCES

- [1] K. N. da Silva, K. Anjanarambath, C. K. W. Lee, H. He, P. Zapol, and P. P. Lopes, “Ir(hkl) Surface Electrochemistry in a Nonadsorbing Acidic Medium,” *Journal of the American Chemical Society* 147 (34), 30708-30722 (2025). DOI: 10.1021/jacs.5c04909.
- [2] D. Y. Chung, P. P. Lopes, P. Farinazzo Bergamo Dias Martins, H. He, T. Kawaguchi, P. Zapol, *et al.*, “Dynamic Stability of Active Sites in Hydr(oxy)oxides for the Oxygen Evolution Reaction,” *Nature Energy* 5, 222-230 (2020).
- [3] P. P. Lopes, D. Y. Chung, X. Rui, H. Zheng, H. He, P. Farinazzo Bergamo Dias Martins, D. Strmcnik, V. R. Stamenkovic, P. Zapol, J. F. Mitchell, R. F. Klie, and N. M. Markovic, “Dynamically Stable Active Sites from Surface Evolution of Perovskite Materials during the Oxygen Evolution Reaction,” *Journal of the American Chemical Society* 143, 2741-2750 (2021).
- [4] D. Hou, H. He, F. Agyapong-Fordjour, Z. Xie, S. Kang, A. Priyadarsini, S. Kattel, P. P. Lopes, P. Zapol, Y. Liu, and G. Li, “Boosting the Oxygen Evolution Reaction by Tuning the Interfacial Iron Adsorption on Layered Double Hydroxide,” *ACS Applied Materials & Interfaces* 17 (28), 41271-41281 (2025).

## Nanoconfined electrolyte-based ionic thermoelectric energy conversion and storage

D. Erts<sup>1\*</sup>, I. Oliseveca<sup>1</sup>, I. L. Leimane<sup>1</sup>, I. Nesterova<sup>2</sup>, G. Kucinskis<sup>3</sup>, R. Meija<sup>1</sup>, R. Poplausks<sup>1</sup>, J. Andzane<sup>1, 1</sup>

1) University of Latvia, Institute of Chemical Physics, Latvia

2) University of Latvia, Institute of Solid State Physics, Latvia

3) Institute of Solid State Physics, University of Latvia, Latvia

\* donats.erts AT lu.lv

Low-grade heat is an abundant yet often underused energy source, requiring innovative materials and device designs to convert small temperature differences into electricity. Ionic thermoelectric systems are gaining attention as promising alternatives to traditional solid-state thermoelectrics because they use low-cost, flexible, and environmentally friendly electrolytes. Nonetheless, their real-world use remains constrained by low power output, sluggish ion dynamics, and limited charge storage.

Ion transport in charged nanochannels differs markedly from conventional Soret diffusion in bulk electrolytes. When a temperature difference is applied across the nanochannels, a gradient in electric double-layer thickness forms, generating an axial electric field that promotes ion separation. This process results in an enhanced potential difference between the hot and cold electrodes.

In this study, sodium-ion thermodiffusion was investigated in aqueous and polymer electrolytes confined within nanoporous matrices, including anodic aluminum oxide, silica aerogels, and silica nanosphere-based structures with varying nanochannel diameters. These nanoporous matrices provide mechanical stability, reduce convective losses, enhance electrolyte retention, and enable the integration of liquid and polymer electrolytes into compact device architectures. Therefore, developing well-defined nanochannels with high surface-to-volume ratios and efficient ion-separation capability is essential for achieving enhanced thermoelectric performance. Moreover, coupling nanoconfined electrolyte systems with intercalation-type electrodes demonstrates their potential not only for thermal energy harvesting but also for charge storage.

Overall, this work highlights nanoconfinement as a powerful and versatile strategy to improve ionic thermoelectric energy conversion and storage. By controlling pore size, surface chemistry, porosity, and electrolyte composition, the thermoelectric response can be systematically tuned, opening new opportunities for efficient waste-heat-to-electricity conversion in low-power, autonomous energy systems.

---

**KEYWORDS:** Ionic thermoelectrics, Nanoconfined electrolyte, Waste heat, Sodium ion intercalation, Thermal energy storage

## The electrocatalytic cracking of polystyrene (PS) using a high-entropy alloy (HEA) anode and janus particles (JP)

K. Kim<sup>1</sup> \*

1) Kyunghee University, Republic of Korea

\* KyuriKim017 AT chiyoulab.org

Traditional methods of catalyzing the conversion of polystyrene to value-added products are costly and not optimized, especially due to incessant coke formation, which leads to a shortened lifespan of catalysts [1]. Thus, the integration of high entropy alloys (HEAs) [2], [3] and Janus particles as a bifunctional catalyst can be a promising method of recovering useful chemicals such as BTX (Benzene, Toluene, Xylene) through enhanced hydrogenolysis and subsequent beta alkyl transfer. Here we investigate the formulation of the FeMnCuCoNi HEA as the anode of the electrocatalytic cell, in which Ni/Fe binary Janus particles are oxidized as a bifunctional catalyst which then act as electrophiles to attack the polystyrene chains. The cathode is composed of RuIr/Ti for traditional Hydrogen Evolution Reaction (HER), which is coupled in an acidic environment using a Bipolar Membrane (BPM). Computational modeling was then used to validate this design and test its function. Through ab initio molecular dynamics (AIMD) simulations, a high degree of polystyrene (PS) adsorption, with a turnover frequency (TOF) of 2.2 s<sup>-1</sup> converted by the Ni/Fe binary Janus particles consequently to being oxidized by the HEA anode. Thus, the high entropy anode along with the Ni/Fe binary Janus particles show particular promise for producing efficient and thus industrially plausible electrocatalysts.

---

**KEYWORDS:** Catalysis, High entropy alloy, Janus particle, AIMD, Polystyrene

---

### REFERENCES

- [1] Z. Xu *et al.*, "Progress and Challenges in Polystyrene Recycling and Upcycling," *ChemSusChem*, vol. 17, no. 17, art. e202400474, 2024.
- [2] X. Feng *et al.*, "High-Entropy Oxide Derived from Metal-Organic Framework for Efficient Oxygen Evolution Reaction," *ACS Appl. Mater. Interfaces*, vol. 15, no. 32, pp. 38164-38175, 2023.
- [3] Q. Li *et al.*, "High-Entropy Metal-Organic Framework ZJU-X100 for Efficient Photocatalytic Applications," *RSC Adv.*, vol. 14, 2024.

## Trivalent europium ion doped WO<sub>3</sub>/WS<sub>2</sub> semiconductor heterostructure interface for efficient hydrogen evolution reaction under acidic and alkaline dual conditions

N. Pachauri<sup>1</sup>\*, V. Mishra<sup>2</sup>, A. Roy<sup>2</sup>, V. Mahalingam<sup>2</sup>, S. Sivakumar<sup>3</sup>

1) IIT Kanpur, India

2) Indian Institute of Science Education and Research Kolkata, India

3) Indian Institute of Technology Kanpur, India

\* namrata.iitk18 AT gmail.com

**Abstract:** Designing economical and efficient electrocatalysts for the hydrogen evolution reaction (HER) in acidic and alkaline dual environments continues to be a critical challenge for sustainable hydrogen generation. Designing electrocatalysts with a high density of electrochemically active sites using simple and scalable synthetic approaches is essential for achieving superior catalytic efficiency. In this context, doping strategies and heterostructure engineering have emerged as an effective approach to enhance catalytic activity by optimizing charge transfer dynamics and increasing active site availability. Here, we have designed the Eu<sup>3+</sup> doped WO<sub>3</sub>-WS<sub>2</sub> semiconductor heterostructure nanomaterials as a cathode for the HER. The material was prepared using a two-step process. First, Eu<sup>3+</sup> doped WO<sub>3</sub> was synthesized by the co-precipitation method and then converted into an oxide-sulfide semiconductor heterostructure using the sulfurization process. The formation of a layered structure, consistently observed in microscopy and supported by phase analysis, is attributed to successful sulfide incorporation. Additionally, the synthesized Eu<sup>3+</sup>:WO<sub>3</sub>/WS<sub>2</sub> semiconductor heterostructure exhibits significant HER performance in both 0.5 M H<sub>2</sub>SO<sub>4</sub> acidic and 1 M KOH alkaline electrolytes, achieving 10 mA cm<sup>-2</sup> current density with corresponding overpotentials of 291 mV vs. RHE and 333 mV vs. RHE, respectively. This significant catalytic behavior is attributed to the synergistic interaction at the heterostructure interface, which enhances charge transfer kinetics and facilitates improved hydrogen evolution in both electrolytes. Moreover, the Eu<sup>3+</sup>:WO<sub>3</sub>/WS<sub>2</sub> heterostructure demonstrates excellent durability, maintaining stable HER performance for 24 hours under acidic conditions and 48 hours in an alkaline environment, highlighting its viability for sustained real-world applications.

**KEYWORDS:** Heterostructures, Electrocatalysis, Interface engineering, Dual-pH catalysis, Rare-earth doping

**ACKNOWLEDGEMENTS:** This work was supported by funding from the Science and Engineering Research Board (SERB/CHE/2021366), Government of India, which the authors gratefully acknowledge.

### REFERENCES

- [1] J. Song, C. Wei, Z. F. Huang, C. Liu, L. Zeng, X. Wang and Z. J. Xu, A review on fundamentals for designing oxygen evolution electrocatalysts, *Chem. Soc. Rev.*, 49, 2196-2214 (2020).
- [2] S. R. Kadam, A. N. Enyashin, L. Houben, R. Bar-Ziv, and M. Bar-Sadan, Ni-WSe<sub>2</sub> nanostructures as efficient catalysts for electrochemical hydrogen evolution reaction (HER) in acidic and alkaline media, *J. Mater. Chem. A*, 8, 1403-1416 (2020).
- [3] H. Liu, M. Jin, D. Zhan, J. Wang, X. Cai, Y. Qiu and L. Lai, Facile synthesis of MoP-Ru<sub>2</sub>P on porous N, P co-doped carbon for efficiently electrocatalytic hydrogen evolution reaction in full pH range, *Appl. Catal., B*, 272, 118951 (2020).
- [4] H. Wang, Y. Cao, C. Sun, G. Zou, J. Huang, X. Kuai, J. Zhao and L. Gao, Strongly Coupled Molybdenum Carbide on Carbon Sheets as a Bifunctional Electrocatalyst for Overall Water Splitting, *ChemSusChem*, 10, 3523 (2017).
- [5] A. I. Inamdar, A. S. Salunke, N. K. Shrestha and H. Im, Heterogeneous oxide/sulfide materials as superior bifunctional electrocatalysts for carbon-neutral green hydrogen production: A short review, *Appl. Phys. Rev.*, 11, 041310 (2024).

## Morphology of nanostructured FeVO<sub>4</sub> layers - a comprehensive study towards improved photoelectrochemical performance

K. Rzepka<sup>1</sup>\*, G. D. Sulka<sup>2</sup>

1) Department of Physical Chemistry and Electrochemistry, Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Krakow, Poland; Doctoral School of Exact and Natural Sciences, Jagiellonian University, Lojasiewicza 11, 30-348 Krakow, Poland., Poland

2) Department of Physical Chemistry and Electrochemistry, Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Krakow, Poland, Poland

\* katarzyna.rzepka AT doctoral.uj.edu.pl

Progressive environmental degradation, rapidly growing energy consumption, and the use of access to fossil fuels as an instrument of economic and political influence are just few prominent examples underscoring the importance of research on advanced technologies for high-efficiency energy generation and effective energy storage. Photoelectrochemical (PEC) water-splitting cells are among the most promising approaches to solar energy conversion, enabling the direct generation of hydrogen without the formation of harmful by-products or additional waste.[1] Despite extensive research on semiconducting photoelectrode materials, controlled doping strategies, and engineered surface architectures, PEC device performance remains limited, primarily due to rapid recombination of photogenerated charge carriers.[2]

Our approach to addressing this issue involves the formation of novel nanostructured heterojunction photoanodes composed of well-established anodic WO<sub>3</sub>[3, 4], coupled with the promising yet still insufficiently explored FeVO<sub>4</sub>, whose bandgap should enable high solar-to-hydrogen conversion efficiency.[5] This contribution reports results from the first stage of this study, aimed at optimizing the morphology of the vanadate layer and examining its influence on photoelectrochemical activity. The application of a straightforward hydrothermal synthesis method, combined with simple manipulation of reaction parameters, allowed us to examine various architectures and identifying approaches best suited to our requirements. A systematic study of nanostructured FeVO<sub>4</sub> for use in PEC water-splitting cells, together with extensive knowledge of anodic WO<sub>3</sub> properties, may represent a new pathway toward the development of advanced devices capable of overcoming detrimental electron-hole recombination. Comprehensive fundamental research, beginning with the investigation of individual component properties, will enable a deeper understanding of the final complex system and help identify the key factors limiting its efficiency.

---

**KEYWORDS:** Photoelectrochemical water splitting, FeVO<sub>4</sub> nanoparticles, Photoanodes, Hydrothermal synthesis

---

**ACKNOWLEDGEMENTS:** The research was carried out under the Opus project financed by the National Science Centre, Poland (no 2025/57/B/ST5/03691). The SEM imaging was performed in the Laboratory of Field Emission Scanning Electron Microscopy and Microanalysis at the Institute of Geological Sciences, Jagiellonian University, Poland.

---

### REFERENCES

- [1] Z. Chen, N. Huyen. Dinh, Eric Miller, Photoelectrochemical Water Splitting. Standards, Experimental Methods, and Protocols. SpringerBriefs in Energy. 2013: Springer New York, NY. 126.
- [2] V. Dhiman, *et al.*, Nanomaterials for photo-electrochemical water splitting: A review. Environmental Science and Pollution Research, 2025. 32(22): p. 13299-13312.
- [3] K. Syrek, *et al.*, The effect of anodization conditions on the morphology of porous tungsten oxide layers formed in aqueous solution. Journal of Electroanalytical Chemistry, 2018. 829: p. 106-115.
- [4] M. Zych, *et al.*, Synthesis and characterization of anodic WO<sub>3</sub> layers in situ doped with C, N during anodization. Electrochimica Acta, 2022. 411: p. 140061.
- [5] S. Chang, *et al.*, FeVO<sub>4</sub> nanopolyhedron photoelectrodes for stable and efficient water splitting. ChemSusChem, 2021. 14(14): p. 3010-3017.

## Shape-directed synthesis of anisotropic gold nanostructures for electrocatalytic oxygen and nitrogen species reduction

S. Zoladek<sup>1\*</sup>, K. Pupil<sup>1</sup>, K. Jędrzejewski<sup>1</sup>, N. Juraev<sup>1</sup>, B. Palys<sup>1</sup>, P. Kulesza<sup>1</sup>

*1) Faculty of Chemistry, University of Warsaw, Poland*

\* szoladek AT chem.uw.edu.pl

The oxygen reduction reaction (ORR) is a key challenge in low-temperature fuel cells due to sluggish kinetics and strong dependence on catalyst composition, morphology, and support effects. Despite efforts to reduce platinum loadings, efficient ORR catalysis still relies on Pt-based systems. Consequently, the development of alternative electrocatalysts exhibiting high activity, selectivity toward the four-electron pathway, and long-term stability is of considerable interest. In parallel, the electrochemical nitrate reduction reaction (NO<sub>3</sub>RR) to ammonia offers a promising route for nitrate remediation, yet is limited by complex multi-electron pathways and competing hydrogen evolution.

In this study, a polyoxometalate-assisted synthetic strategy is employed to control the anisotropy of gold nanostructures as well as the sphericity of gold nanoparticles immobilized on carbon-based supports at low metal loadings. Keggin-type polyoxometalates act as inorganic reducing, stabilizing, and shape-directing agents, enabling surfactant-free synthesis without conventional organic ligands such as PVP, amines, thiols, or surfactants, which block active sites and alter intrinsic catalytic properties. Precise morphology control is achieved by tuning nucleation and growth kinetics through the combined use of mixed reducing agents, gold precursors, polyoxometalates, and silver ions. This enables the formation of anisotropic nanoplates (triangular and hexagonal), nanorods, nanostars, nanoflowers, nanourchins, as well as hollow and concave architectures such as nanobowls and donut-like nanostructures formed via galvanic replacement. In parallel, highly dispersed spherical gold nanoparticles are deposited on carbon-based supports.

Spectroscopic (UV-Vis, FTIR), microscopic (SEM, TEM), and structural (XRD) analyses confirm stabilization of nanostructures during synthesis and removal of polyoxometalate layers under alkaline conditions without altering morphology. Electrochemical diagnostics using cyclic voltammetry and rotating ring-disk electrode (RRDE) measurements reveal pronounced morphology- and support-dependent effects on ORR activity and selectivity. In particular, spherical gold nanoparticles supported on carbon-based supports exhibit low peroxide yields and electron transfer numbers approaching four, indicating a dominant four-electron ORR pathway. Anisotropic nanostructures show distinct activity trends associated with their high density of low-coordinated surface atoms and defect-rich surfaces. Additionally, the materials exhibit enhanced performance toward NO<sub>3</sub>RR, favoring multi-electron reduction pathways toward ammonia.

---

**KEYWORDS:** Oxygen reduction reaction (ORR), Nitrate reduction reaction (NO<sub>3</sub>RR), Gold nanostructures, Anisotropic nanoparticles, Rotating Ring-Disk electrode (RRDE)

## Posters

T4-10

POSTER

### Testing the performance of sea water batteries with solid electrolyte nasicon-type in the presence of recirculated CO<sub>2</sub>

A. Marinoiu<sup>1\*</sup>, M. Iordache<sup>2</sup>, V. Podhurska<sup>3</sup>

1) Institute for Cryogenics and Isotopic Technologies - ICSI, Ramnicu Valcea, Romania, Romania

2) National Research and Development Institute for Cryogenic and Isotopic Technologies - ICSI Ramnicu Valcea, Romania, Romania

3) Karpenko Physico-Mechanical Institute of the National Academy of Sciences of Ukraine, Ukraine

\* adriana.marinoiu AT icsi.ro

The abundance and durability of renewable natural resources have drawn attention to their use as energy sources. Rechargeable seawater batteries (SWBs) are considered sustainable alternatives to Li-ion batteries due to the use of an unlimited and free source of Na-ion active materials. SWB systems not only benefit from the unlimited source of active materials, but also, thanks to their unique design with the open cathode structure, they significantly manage the heat circulation of the system to ensure safety and longer service life. Seawater Na-CO<sub>2</sub> technologies offer a promising framework for the development of integrated „seawater" systems capable of combining energy storage with CO<sub>2</sub> capture or recovery. In this study, testing experiments were carried out to evaluate the functioning of a NASICON membrane seawater battery cell in the presence of recirculated CO<sub>2</sub>. Experiments with CO<sub>2</sub> recirculation have highlighted the complex interaction between sodium storage processes and secondary reactions from the aqueous environment, in particular the evolution of hydrogen (HER). Chromatographic analyses confirmed the formation of H<sub>2</sub> (values between  $2.42 \times 10^{-3}$  and  $3.9 \times 10^{-3}$  mL·min<sup>-1</sup>), and the values of faradaic efficiency (approx.20%) indicate a competition between the target reactions (associated to the CO<sub>2</sub> conversion and/or redox processes of the battery) and the parasitic reactions. The stability of tensions in some regimens and the variation of faradaic efficiency over time suggest that the system is sensitive to local pH conditions, the accumulation of carbonate/bicarbonate species and the nature of the catalyst used (Pt/C). These results validate the functionality of the concept, but also highlight clear directions for optimisation, in particular on catalytic selectivity and reduction of polarisation.

**KEYWORDS:** Seawater batteries, NASICON membrane, CO<sub>2</sub> conversion, Redox processes

**ACKNOWLEDGEMENTS:** National Authority for Scientific Research (Romania) (ANCS) provided financial support for this work through the projects PN 23 15 01 03 and PN 23 15 01 04, Contract no. 20N/2023 and by the project RO-HydroHub “Romanian Hydrogen and New Energy Technologies Hub”, contract nr. G2025-113330/ 2025, SMIS code: 351358, financed from European funds via the POCIDIF 2021-2027 Program.

## Raman-correlated electrocatalytic H<sub>2</sub>O<sub>2</sub> sensing at fragmented graphene Oxide/Gold nanourchin hybrid

K. Pupał<sup>1</sup>\*, S. Zoladek<sup>1</sup>, B. Palys<sup>1</sup>

*1) Faculty of Chemistry, University of Warsaw, Poland*

\* k.pupał AT uw.edu.pl

Electrochemical detection of hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>) is essential for monitoring oxidative processes in biological, environmental and technological systems. In this work, we develop non-enzymatic H<sub>2</sub>O<sub>2</sub> sensors based on hybrid layers composed of graphene oxide-related materials and anisotropic gold nanostructures. Our previous study showed that the morphology of gold nanoparticles and the defect structure of graphene oxide (GO) strongly influence the electrocatalytic reduction of H<sub>2</sub>O<sub>2</sub>. Among gold nanospheres, nanobowls and nanourchins (AuNURs), the nanourchin morphology provided the highest amperometric response, especially after coupling with electrochemically reduced graphene oxide (ERGO), due to the combination of a highly developed gold surface, sharp edges, and improved charge transport in the carbon layer [1].

Here, we extend this concept by introducing fragmented graphene oxide (fGO) and electrochemically reduced fragmented graphene oxide (ERfGO) as supports for gold nanourchins. Fragmentation is used as a structural strategy to increase the density of exposed edges, defects and accessible oxygen-containing sites, while reducing diffusion limitations within the hybrid sensing layer. The materials are deposited on glassy carbon electrodes and characterized by electron microscopy, Raman spectroscopy and electrochemical methods. The amperometric response toward H<sub>2</sub>O<sub>2</sub> is evaluated in phosphate buffer at near-neutral pH, and the sensor performance is correlated with Raman parameters describing disorder, graphitic domains and oxygen-related structural features.

The fGO/AuNURs hybrids exhibit enhanced sensitivity compared with analogous non-fragmented GO-based layers. The effect is further amplified after electrochemical reduction, indicating that the most favourable sensing architecture requires a balance between defect density, accessible adsorption sites and electrical conductivity. Raman analysis supports this interpretation: an increased contribution of defect-related bands, together with preservation of conductive carbon domains, accompanies the improved H<sub>2</sub>O<sub>2</sub> reduction currents. These results confirm that fragmentation of graphene oxide is not only a morphological modification but also an effective route to tune the electrocatalytic interface.

The study highlights the synergistic role of GO defects and AuNURs morphology in non-enzymatic peroxide sensing. The proposed fragmented ERfGO/AuNURs platform offers a promising pathway toward highly sensitive, stable and enzyme-free electrochemical sensors for hydrogen peroxide and related reactive oxygen species.

---

**KEYWORDS:** Graphene oxide, Gold nanoparticles, Raman spectroscopy, Electrocatalysis, Hydrogen peroxide

---

**ACKNOWLEDGEMENTS:** This project is funded by the Research University - Excellence Initiative program: 501-D112-20-0004410

---

### REFERENCES

- [1] K. Pupał, K. Jędrzejewski, S. Zoladek, M. Palys, B. Palys, The graphene oxide/gold nanoparticles hybrid layers for hydrogen peroxide sensing-Effect of the nanoparticles shape and importance of the graphene oxide defects for the sensitivity. *Molecules*, 30(3), 533 (2025).

## Electrochemical control of chloramphenicol adsorption at gold nanostructures using EC-SERS

K. Jędrzejewski<sup>1</sup>\*, B. Palys<sup>1</sup>

*1) Faculty of Chemistry, University of Warsaw, Poland*

\* kk.jedrzejewski AT uw.edu.pl

Nanostructured noble-metal electrodes provide a versatile platform for studying molecular processes at electrochemical interfaces, particularly when optical signal amplification is combined with potential control. In this work, gold nanoparticle-modified screen-printed electrodes were used as model nanostructured interfaces for investigating the electrochemical adsorption behavior of chloramphenicol, a broad-spectrum antibiotic of environmental and analytical relevance.

Electrochemical surface-enhanced Raman spectroscopy (EC-SERS) was applied to monitor potential-dependent changes occurring at the gold/electrolyte interface in phosphate buffer solution. By varying the electrode potential, the interfacial conditions were tuned in a controlled manner, allowing changes in the adsorption state of chloramphenicol to be followed through its enhanced vibrational response. The recorded spectra show characteristic bands related to the aromatic moiety and functional groups of the molecule, while their relative intensities depend strongly on the applied potential. These changes indicate that the electric field at the nanostructured gold surface affects both the adsorption configuration of chloramphenicol and the efficiency of Raman signal enhancement.

The results demonstrate that gold nanoparticle-modified electrodes can serve not only as signal-enhancing substrates, but also as electrochemically tunable nanointerfaces for probing molecular adsorption phenomena. This approach provides insight into charge-transfer and adsorption-related processes at plasmonic metal nanostructures and supports the rational development of electrochemical-spectroscopic sensing platforms for antibiotic residue detection.

---

**KEYWORDS:** EC-SERS, Raman, Chloramphenicol, Gold nanoparticles

## Low-temperature precipitation synthesis of $\text{Na}_3\text{V}_2\text{O}_x(\text{PO}_4)_2\text{F}_{3-x}$ nano- and microparticles with tunable morphology for sodium-ion battery cathodes

O. Grabowski<sup>1\*</sup>, M. Krajewski<sup>1</sup>, M. Winkowska-Struzik<sup>1</sup>, A. Czerwiński<sup>1</sup>

*1) Faculty of Chemistry, University of Warsaw, Poland*

\* o.grabowski AT uw.edu.pl

Sodium-ion batteries have emerged as a promising alternative to lithium-ion systems due to the natural abundance, low cost, and wide geographical distribution of sodium resources[1]. Among the various cathode materials investigated, sodium vanadium fluorophosphates (NVPF,  $\text{Na}_3\text{V}_2\text{O}_x(\text{PO}_4)_2\text{F}_{3-x}$ , where  $0 \leq x \leq 2$ ) have attracted particular attention owing to their high operating voltage (ca. 3.8-3.9 V vs  $\text{Na}^+/\text{Na}^0$ ), robust structural stability, high theoretical specific capacity (ca. 128 mAh  $\text{g}^{-1}$ ) and favorable  $\text{Na}^+$  diffusion pathways[2]. These features make them strong candidates for post-lithium energy storage systems.

In this work,  $\text{Na}_3\text{V}_2\text{O}_x(\text{PO}_4)_2\text{F}_{3-x}$  materials were synthesized via a precipitation method under a variety of controlled conditions, including variations in temperature, pH, use of surfactants and solvent modifications. The synthesis involved the use of a reducing agent not previously reported for NVPF preparation. Importantly, the obtained materials crystallize directly from solution in the desired phase without the need for high-temperature calcination, highlighting the efficiency and scalability of the method. By systematically tuning these parameters, both nano- and microparticles with diverse and distinctive morphologies were obtained. Notably, a unique hierarchical morphology resembling pinecone-like structures was achieved, offering increased surface area and potentially enhanced electrochemical accessibility. The resulting materials were comprehensively characterized using scanning electron microscopy and powder X-ray diffraction, while their electrochemical performance in Na-ion cells was evaluated in terms of high-rate capability and cycling stability. The best-performing materials delivered a high specific capacity close to 120 mAh  $\text{g}^{-1}$  at a current rate of 0.1 C and retained over 95% of their capacity after 100 cycles at 2 C.

This study demonstrates that precipitation synthesis of NVPF using a proposed reducing agent is a versatile approach for obtaining particles with tunable morphology and favourable electrochemical performance.

---

**KEYWORDS:** Sodium-Ion batteries, Cathode material synthesis, Sodium vanadium fluorophosphate (NVPF), Precipitation synthesis

---

**ACKNOWLEDGEMENTS:** This work was supported by The Polish National Centre of Science through a research grant 2025/57/N/ST5/04686 entitled "Amorphous transition metal phosphates as positive electrode materials for sodium-ion batteries".

---

### REFERENCES

- [1] N. Yabuuchi, K. Kubota, M. Dahbi, S. Komaba, "Research Development on Sodium-Ion Batteries" *Chem. Rev.*, 114, 23, 11636-11682 (2014).
- [2] R. Fang, J. Olchowka, C. Pablos, R. B. Nuernberg, L. Croguennec, S. Cassaignon, "Impact of the F - for O 2- Substitution in  $\text{Na}_3\text{V}_2(\text{PO}_4)_2\text{F}_{3-y}\text{O}_y$  on Their Transport Properties and Electrochemical Performance", *ACS Appl. Energy Mater.*, 5, 1, 1065-1075 (2022).

## Effect of synthesis conditions on morphology of Cu-doped lithium-nickel oxide for cobalt-free lithium-ion batteries

M. Grygiel<sup>1\*</sup>, F. Lemiesz<sup>2</sup>, H. Ronduda<sup>2</sup>, B. Hamankiewicz<sup>1</sup>, M. Winkowska-Struzik<sup>1</sup>, M. Krajewski<sup>1</sup>,  
A. Czerwiński<sup>1</sup>

1) Faculty of Chemistry, University of Warsaw, Poland

2) Warsaw University of Technology, Poland

\* mm.grygiel2 AT uw.edu.pl

The development of high-energy-density, cobalt-free cathode materials is a critical priority for the next generation of lithium-ion batteries due to the economic and environmental concerns associated with cobalt.[1] Lithium nickel oxide (LiNiO<sub>2</sub>, LNO) is a primary candidate for these applications, offering a high theoretical specific capacity of 275 mAh g<sup>-1</sup>, which is comparable to current nickel-manganese-cobalt (NMC) technologies. [2] However, LNO suffers from significant structural instability caused by the disordering of lithium and nickel atoms, a phenomenon known as “cation mixing” resulting from the similar ionic radii of Li<sup>+</sup> and Ni<sub>2+</sub>.[3] Furthermore, multiple phase transitions during lithium intercalation induce mechanical strain, leading to particle cracking and surface deterioration.[4]

This study investigates the effect of particle size and morphology of copper-doped LNO to enhance the structural and electrochemical stability of this material. Copper was selected due to its similar ionic radius to Li<sup>+</sup> and Ni<sub>2+</sub> ions, what enables the potential for stabilization of crystal lattice.[5] Copper is also highly available worldwide, low cost, and can be sourced from recycling. The research specifically compares two distinct precursor synthesis methodologies for tailoring particle characteristics: a solid-state mechanochemical route utilizing high-energy ball-milling and a co-precipitation method. The synthesized precursors were calcined with lithium hydroxide under oxygen atmosphere to promote formation of a well-ordered layered crystal structure.

The physicochemical properties of the resulting materials were characterized using X-ray powder diffraction with Rietveld refinement to determine phase purity and the degree of cation disordering. Additionally, morphological analysis via electron microscopy and surface area determination through N<sub>2</sub> adsorption method (BET) were conducted to correlate synthesis parameters with particle distribution. Electrochemical performance was evaluated in half-cell configurations against metallic lithium, focusing on specific capacity and capacity retention.

X-ray diffraction studies demonstrate successful formation of Cu-enriched phase (LiNi<sub>1-x</sub>Cu<sub>x</sub>O<sub>2</sub>). Comparative analysis of SEM images and BET results indicates that the synthesis route significantly influences the final size distribution of material particles, which is a crucial parameter to optimize for high-rate electrochemical performance in lithium-ion setup.

---

**KEYWORDS:** Lithium-ion batteries, Cathode materials, Lithium-nickel oxide, Copper-doping, Energy storage

---

**ACKNOWLEDGEMENTS:** This research was funded by the National Science Centre, Poland, under grant number 2025/57/B/ST5/03718.

---

### REFERENCES

- [1] Nitin Muralidharan *et al.*, Adv. Energy Mater. (2022) 12, 9, 2103050
- [2] Dongsoo Lee *et al.*, Adv. Energy Mater. (2024) 14, 19, 2303490
- [3] Rio Akbar Yuwono *et al.*, Chem. Eng. J. (2023) 456, 141065
- [4] Barbara Nascimento Numes *et al.*, ChemSusChem (2024) 18, 8, e202402202
- [5] Xiang-Ze Dong *et al.*, J. Electrochem. Soc. (2020) 167, 140545

# Track 5

## Multifunctional Thin Films and Advanced Coatings

## Cu-driven structural evolution of layered chalcogenide thin films towards Cu-rich telluride nanostructures

A. Lotnyk<sup>1</sup>\*, N. Braun<sup>1</sup>, V. Roddatis<sup>2</sup>, D. Kalanov<sup>1</sup>, M. Rudolph<sup>1</sup>, L. Voss<sup>3</sup>, S. Cremer<sup>1</sup>, L. Kienle<sup>3</sup>

1) Leibniz Institute of Surface Engineering (IOM), Germany

2) GFZ Helmholtz Centre for Geosciences, Germany

3) Institute for Materials Science, Faculty of Engineering, University of Kiel, Germany

\* andriy.lotnyk AT iom-leipzig.de

Copper tellurides are promising materials for thermoelectric [1] and memory technologies, [2] yet their functional properties are governed by atomic-scale structure, defects, and phase evolution that remain insufficiently understood. In this talk, I will discuss complementary studies on Cu-driven structural evolution in layered chalcogenide thin films [3] and on the atomic-scale structure of Cu-rich telluride nanostructures [4].

Starting from epitaxial  $\text{Sb}_2\text{Te}_3$ , room-temperature magnetron sputtering of Cu triggers interdiffusion and the formation of disordered Cu-Sb-Te nanolayers within the layered host [3]. The extent of this transformation depends strongly on sputtering pressure: lower Ar pressure increases the kinetic energy of incoming Cu species, enhances Cu incorporation, expands the  $\text{Sb}_2\text{Te}_3$  lattice, and promotes Cu-Sb-Te formation. Monte Carlo simulations support this interpretation by showing that gas-phase scattering suppresses the high-energy fraction of the Cu flux at higher pressure. Further metal deposition drives a nearly complete conversion of  $\text{Sb}_2\text{Te}_3$  into a previously unreported  $\text{Cu}_7(\text{Sb}_{0.4}\text{Te}_{0.6})_4$  phase. Atomic-resolution scanning transmission electron microscopy (STEM), combined with chemical analysis and image simulations, reveals an epitaxial layered structure dominated by 3 Te building units, but also containing 2 Te units, Sb/Te antisite defects, and Cu vacancies. These observations enable a structural model for a layered hexagonal phase that is related to, yet distinct from, known trigonal  $\text{Cu}_7\text{Te}_4$  polymorphs. Upon thermal treatment, Sb out-diffuses and oxidizes, while the Cu-Sb-Te phase transforms into layered  $\text{Cu}_7\text{Te}_4$ .

In a complementary atomic-scale study of thermally reacted Cu/ $\text{Sb}_2\text{Te}_3$ -based systems prepared from thicker  $\text{Sb}_2\text{Te}_3$  films, the as-formed layered  $\text{Cu}_7\text{Te}_4$  nanostructures were resolved in detail by aberration-corrected STEM [4]. Two related trigonal configurations composed of distorted close-packed Te layers separated by vacancy layers were identified: a double-layered structure with 2 Te layers per nanoscale building unit and a triple-layered structure with 3 Te layers per unit. While the double-layered configuration is consistent with established models, the triple-layered  $\text{Cu}_7\text{Te}_4$  represents a newly identified structural variant that can occur in both ordered and Cu-vacancy-disordered forms. Both structures exhibit stacking faults, twin boundaries, dislocations, and local transition regions, demonstrating that short-range rearrangements of the Cu sublattice, together with subtle Te displacements, enable structural conversion between the two motifs.

Together, these studies provide a coherent picture of Cu-driven evolution from  $\text{Sb}_2\text{Te}_3$  to defect-rich layered  $\text{Cu}_7\text{Te}_4$  via metastable Cu-Sb-Te phases and show how atomic-scale disorder and nanoscale building units can be exploited to tailor chalcogenides for thermoelectric and memory applications [5].

---

**KEYWORDS:** Thin films, Layered chalcogenides, Copper tellurides, Phase transformation, Structure analysis

---

**ACKNOWLEDGEMENTS:** The authors thank A. Mill for TEM lamella preparation, H. Bryja for the growth of epitaxial  $\text{Sb}_2\text{Te}_3$  thin films as well as T. Pröhl and P. Hertel for DC magnetron sputtering. We acknowledge the financial support by the German Research Foundation (DFG 448667535). The authors thank the European Regional Development Fund and the State of Brandenburg for the Themis Z microscope (part of the Potsdam Imaging and Spectral Analysis (PISA) facility).

---

### REFERENCES

- [1] Y. He, T. Zhang, X. Shi, S.-H. Wei, L. Chen, High thermoelectric performance in  $\text{Cu}_2\text{Te}$ . *NPG Asia Mater.*, 7, e210 (2015).
- [2] L. Yin, R. Cheng, S. Pan, W. Xiong, S. Chang, B. Zhai, Y. Wen, Y. Cai, Y. Guo, M. G. Sendeku, J. Jiang, W. Liao, Z. Wang, J. He, Engineering Atomic-Scale Patterning and Resistive Switching in 2D Crystals and Application in Image Processing. *Adv. Mater.*, 35, 306850 (2023)
- [3] N. Braun, D. Kalanov, M. Rudolph, V. Roddatis, L. Voß, S. Cremer, H. Bryja, L. Kienle, A. Lotnyk, Synthesis and microstructural characterization of layered Cu-Sb-Te-based thin films, *Appl. Surf. Sci. Adv.* 31, 100911 (2026)
- [4] A. Lotnyk, V. Roddatis, N. Braun, L. Voß, H. Bryja, L. Kienle, Atomic-Scale Investigation of Layered  $\text{Cu}_7\text{Te}_4$  Nanostructures Featuring Two and Three Tellurium Layers, *ACS Appl. Nano Mater.* 8, 11621-11628 (2025)
- [5] S. Yan, D. Cai, Y. Xue, T. Guo, S. Song, Z. Song, Sb-rich  $\text{CuSbTe}$  material: A candidate for high-speed and high-density phase change memory application, *Mater. Sci. Semicond. Process.*, 103, 104625 (2019)

## Interpretable Grey-Box AI for Plasma-Deposited thin films in the era of EUV lithography

Y. Wakabayashi<sup>1</sup>, K. Kamataki<sup>2</sup>, M. Hatashita<sup>1</sup>, T. Yamamoto<sup>1</sup>, M. Shiratani<sup>2</sup>\*

1) SPP Technologies Co., Ltd., Japan

2) Kyushu University, Japan

\* siratani AT ed.kyushu-u.ac.jp

The introduction of extreme ultraviolet (EUV) lithography has placed stringent requirements on plasma-deposited thin films used in advanced semiconductor manufacturing, including dielectric layers, hard masks, and functional nanocoatings. At EUV-relevant dimensions, thin-film growth is governed by complex and strongly coupled plasma-surface interactions, where nanoscale structural uniformity, stress, and defect control become critical challenges [1-3].

In this invited talk, we present an interpretable grey-box artificial intelligence (AI) framework for plasma-deposited thin films, designed to meet the demands of the EUV lithography era. The framework integrates plasma physics, materials science, and data science by combining machine learning with physically grounded descriptors derived from plasma diagnostics. In particular, we employ plasma-material information science (PaMIS) to construct features from optical emission spectroscopy (OES) that are causally linked to thin-film growth and properties, rather than relying solely on external process parameters [4, 5].

Explainable machine-learning techniques are incorporated to identify key plasma species and reaction pathways governing deposition kinetics and materials evolution, enabling mechanistic insight beyond black-box optimization. Furthermore, diversity metrics originally developed in statistical physics are introduced to quantify plasma chemical diversity and to relate it to variations in thin-film structure and stress at the nanoscale. This analysis reveals that plasma-state diversity plays a decisive role in stabilizing thin-film growth and controlling material variability under EUV-relevant conditions.

The proposed grey-box AI approach provides a data-efficient and physically interpretable methodology for accelerating R&D of plasma-deposited thin films. By preserving scientific insight while leveraging AI, it offers a scalable pathway for materials design and process control in next-generation EUV lithography.

---

**KEYWORDS:** Thin film, Plasma process, Machine learning, OES

---

**ACKNOWLEDGEMENTS:** This work was partly supported by JSPS KAKENHI (Grant No. 26K00692 , No. JP24H00205 and No. JP23K03368) and JST ASPIRE (Grant No. 1234505).

---

### REFERENCES

- [1] K. J. Kanarik, Inside the mysterious world of plasma: A process engineer’s perspective, *J. Vac. Sci. Technol. A*, 38, 031004 (2020).
- [2] I Adamovich, *et al.*, The 2022 Plasma Roadmap: low temperature plasma science and technology, *J. Phys. D*, 55, 373001 (2022).
- [3] H. Mizoguchi, *et al.*, EUV exposure for photo-chemical materials and LPP-EUV source research for semiconductor manufacturing, *Optical and EUV Nanolithography XXXIX*, 13979, 1397913 (2026).
- [4] S. W. Fitriani, K. Kamataki, Y. Yamamoto, Y. Sato, Y. Kurosaki,, K. Koga, and M. Shiratani, Predictive model for SiO<sub>2</sub> film properties using plasma optical emission spectra based on machine learning, *Surface & Coatings Technology*, 504, 132029 (2025).
- [5] M. Shiratani, S. W. Fitriani, and K. Kamataki, Accelerating Research and Development through Grey-Box Approaches and Diversity Metrics in Plasma Processes, *Proc. 43rd Symposium of Plasma Processing*, 4 (2026).

## Plasma-assisted synthesis of hybrid nanomaterials for enhanced SERS performance

O. Kylian<sup>1</sup>\*, P. Pivko<sup>1</sup>, M. Pavlović<sup>1</sup>, J. Hanuš<sup>1</sup>, E. Kočišová<sup>2</sup>, M. Procházka<sup>2</sup>

1) Charles University, Faculty of Mathematics and Physics, V Holešovičkách 2, 180 00 Prague 8, Czech Republic, Czech Republic

2) Charles University, Faculty of Mathematics and Physics, 121 16, Prague 2, Czech Republic, Czech Republic

\* ondrej.kylian AT matfyz.cuni.cz

Surface-enhanced Raman scattering (SERS) spectroscopy has emerged as an indispensable tool for molecular detection, with applications ranging from forensics or food quality control to pharmaceutical development or medical applications [1]. While traditional SERS platforms rely on the electromagnetic enhancement of noble metal nanostructures (Au, Ag, or Cu), recent advancements have highlighted the potential of non-plasmonic materials, such as metal oxides and certain conducting polymers [2-5]. These materials, whose SERS performance is primarily due to a chemical enhancement mechanism via photo-induced charge transfer, often offer superior stability and lower costs, though they typically exhibit lower SERS activity than their metallic plasmonic counterparts. From an application standpoint, the trade-off between high sensitivity and chemical stability remains a significant challenge. This study addresses this gap by utilising plasma-assisted deposition techniques to engineer advanced SERS-active hybrid metal-metal oxide and metal-polymer coatings. The experimental strategy involved the controlled decoration of various substrates with sputter-deposited plasmonic metal nanostructures (Ag or Au), including:

- Metal oxide films prepared by magnetron sputtering or metal oxide nanoparticles synthesised via magnetron-based gas aggregation sources
- Polymeric films (quaterthiophene) deposited through plasma-assisted vacuum thermal evaporation.

Comprehensive analysis reveals that coating composition and morphology are in all cases critical to SERS performance. Furthermore, it is shown that under optimised conditions, these heterostructures yield signal enhancements that exceed those of pure plasmonic, metal oxide, or polymeric materials. Notably, in systems involving TiO<sub>2</sub>, Nb<sub>2</sub>O<sub>5</sub>, or WO<sub>3</sub>, the produced heterostructures also exhibit UV-induced recyclability, adding a layer of multi-functionality. These findings provide a novel pathway for developing advanced, stable, highly sensitive, and robust SERS sensors.

---

**KEYWORDS:** SERS, Plasma-assisted deposition, Hybrid nanomaterials

---

**ACKNOWLEDGEMENTS:** The authors thank the Czech Science Foundation (grant No. 24-12197S) for financial support.

---

### REFERENCES

- [1] M. Procházka, „Surface-Enhanced Raman Spectroscopy“, Springer, Cham (2016)
- [2] X. Du, D. Liu, K. An, S. Jiang, Z. Wei, S. Wang, W.F. Ip, and H. Pan, „Advances in oxide semiconductors for surface enhanced Raman scattering“, *Appl. Mater. Today*, 29, 101563 (2022)
- [3] E. Kočišová, O. Kylián, and M. Procházka, „Non-plasmonic Metal Oxide Nanostructures for SERS Applications“. In: M. Procházka, J. Kneipp, B. Zhao, Ozaki, Y. (eds) *Surface- and Tip-Enhanced Raman Scattering Spectroscopy*. Springer, Singapore (2024)
- [4] M. Yilmaz, E. Babur, M. Ozdemir, R.L. Gieseck, Y. Dede, U. Tamer, G.C. Schatz, A. Facchetti, H. Usta, and G. Demirel, „Nanostructured organic semiconductor films for molecular detection with surface-enhanced Raman spectroscopy“, *Nat. Mater.*, 16, 918-924 (2017)
- [5] G. Demirel, R.L.M. Gieseck, R. Ozdemir, S. Kahmann, M.A. Loi, G.C. Schatz, A. Facchetti, and H. Usta, “Molecular engineering of organic semiconductors enables noble metal-comparable SERS enhancement and sensitivity”, *Nat. Commun.*, 10, 5502 (2019)

## High-throughput manufacturing of 2D nanomaterial coatings on polymer films for flexible electronic applications

I. Luzinov<sup>1</sup>\*

*1) Department of Material Science and Engineering, Clemson University, USA*

\* luzinov AT clemson.edu

Scalable nanomanufacturing of two-dimensional (2D) materials coating on polymer substrates remains a critical challenge for flexible electronic systems. Current approaches often require multistep processing, harsh surface treatments, or are incompatible with continuous manufacturing. To this end, we report a water-based, high-throughput dip-coating strategy for the direct deposition of graphene oxide (GO) and related 2D nanomaterials onto hydrophobic polymer films without surface pre-treatment. The process employs amphiphilic reactive macromolecular super-spreaders (RMS) that conformally encapsulate GO sheets. This modification enables thermodynamically driven, interface-directed assembly of uniform nanoscale layers on low-energy polymer surfaces. Our method allows accurate control of coating thickness, from single layers to multilayer films. It is achieved by tuning the RMS composition, suspension concentration, and withdrawal rate. Subsequent chemical reduction yields conductive reduced graphene oxide (rGO) coatings with conductivities approaching  $\sim 10^3$  S/cm. The films exhibit high optical transparency and strong adhesion to polymer substrates, such as polypropylene, polycarbonate, and Kapton. Electro-mechanical testing shows stable electrical performance under repeated bending, with minimal degradation after cyclic deformation. The process is continuous, scalable, and compatible with industrial coating techniques. It avoids toxic solvents and aggressive surface modification steps. This improves environmental compatibility and manufacturing efficiency. Our approach can be applied to other 2D materials, including transition-metal dichalcogenides and MXenes. It can, thus, enable the fabrication of heterogeneous multilayer assemblies with tunable electronic properties. In conclusion, this work establishes a direct link between processing conditions, nanoscale structure, and functional properties of 2D coatings on flexible substrates. It provides a versatile and scalable nanomanufacturing framework for integrating diverse 2D materials into next-generation flexible and wearable electronic devices.

---

**KEYWORDS:** Graphene oxide, Conductive coatings, Flexible electronics, Polymer films, 2D materials

## Well-defined molecular films as a platform for probing molecular properties on the surface

F. Nishino<sup>1\*</sup>, T. K. Yamada<sup>2</sup>, S. Kera<sup>3</sup>

1) National Institutes for Quantum Science and Technology (QST), Japan

2) Chiba University, Japan

3) Institute for Molecular Science, Japan

\* nishino.fumi AT qst.go.jp

Well-defined two-dimensional (2D) thin films consist of complex molecules, such as stimuli responsive molecules and chiral molecules, are recognized as effective platforms for investigating molecule-substrate interfaces and single-molecule functions [1,2].

For example, it is well known that the 2D-crystallization of chiral molecules on achiral substrates can transfer chirality to the surface. In such systems, the giant spin polarization phenomena associated with chiral molecular ordering, which is known as chirality-induced spin selectivity (CISS), have been reported and are actively studied.

On the other hand, formation of molecular films is based on relatively weak interactions compared to inorganic materials, resulting in a high degree of structural freedom and often leading to complex ordered structures and structural instability [3]. As a result, there are limited studies in which the relationship between detailed structural characterization at interfaces and the resulting functional properties has been examined.

In this presentation, to precisely determine the ordered structures of molecular films and elucidate the relationship between the molecular ordering and its properties, we used scanning tunneling microscopy (STM), scanning tunneling spectroscopy (STS), and distortion-corrected low-energy electron diffraction (LEED) [4]

First, we fabricated on ferrocene-based molecular complexes periodically arranged on a crown ether monolayer. We observe reversible molecular motion induced by voltage application and discuss the nanoscale sliding motion of molecule originating from the modulation of intermolecular interactions [5]. Second, we examine the two-dimensional crystallization of chiral molecules on achiral substrates. In this study, helicene molecules with a helical structure are adsorbed onto an Au substrate, and their ordered structures are carefully characterized. Based on these observations, we experimentally demonstrate that mirror-imaged growth governed by substrate symmetry can also occur in systems without commensurability [6]. These two studies suggest that precise definition of ordered structures in complex molecular systems provides new insights into molecular unique properties.

---

**KEYWORDS:** Surface science, Organic thinfilms, Chirality, Stimuli-responsive molecule

---

**ACKNOWLEDGEMENTS:** I would like to acknowledge valuable collaborations with K. Fukutani and S. Kera (Institute for Molecular Science), J. Brandhoff, E. Fuerch, F. Otto, M. Grünwald, M. Schaal, R. Forker, D. Stelter, T. Fritz, J. Picker, and A. Turchanin (Friedrich Schiller University Jena), Z. Zhang and T. Hirose (Kyoto University), P. Krüger and T. K. Yamada (Chiba University), C.-H. Wang, Y.-H. Chang (National Tsing Hua University), M. Horie (Hokkaido University), R. Nemoto (Science Tokyo), T. Hosokai (National Institute of Advanced Industrial Science and Technology), and Y. Hasegawa (University of Tsukuba) for their significant contributions to this study.

---

### REFERENCES

- [1] J. Teyssandier *et al.*, Chem. Commun. 52, 11465 (2016).
- [2] K. Ernst, Phys. status solidi 249, 2057 (2012).
- [3] R. Forker, M. Meissner, and T. Fritz, Soft Matter 13, 1748 (2017).
- [4] F. Sojka *et al.*, Rev. Sci. Instrum. 84, (2013).
- [5] F. Nishino *et al.*, Small 21, 1 (2025).
- [6] F. Nishino *et al.*, Appl. Phys. Express 18, 015502 (2025).

## Implementation of high-performance superlattice-like phase-change memory via sputtering deposition

H. Sung<sup>1\*</sup>, S. Kim<sup>1</sup>, H. Lee<sup>1</sup>

*1) Korea University, Republic of Korea*

\* sunghansang AT gmail.com

As the demand for next-generation storage class memory (SCM) with high-speed and low-power characteristics intensifies, phase-change memory (PCM) has emerged as a promising technology. However, conventional Ge-Sb-Te (GST)-based devices continue to face persistent challenges, such as excessive power consumption and degraded thermal stability during aggressive scaling. To address these bottlenecks, this study proposes a synergistic approach that integrates strategic material doping with a superlattice-like (SLL) architecture to maximize device switching performance.

First, we developed a Ta-doped Sb<sub>2</sub>Te<sub>3</sub> (TST) materials designed to enhance both amorphous and thermal stability [1]. The incorporation of Ta atoms into the Sb<sub>2</sub>Te<sub>3</sub> matrix effectively accelerates crystallization speed while suppressing grain growth, thereby mitigating the resistance drift and spontaneous data loss common in traditional chalcogenides. This doping strategy ensures a sufficient thermal margin, enabling reliable phase-transition control and superior data retention even in high-temperature environments.

From a nano-structural perspective, the optimized TST material was interleaved with TiTe<sub>2</sub> (TT) layers to realize an SLL configuration [2]. By fine-tuning the sputtering parameters, we optimized the fabrication of high-quality SLL films. Structural analysis via XRD and HR-TEM confirmed well-aligned c-plane growth and the formation of distinct van der Waals gaps at the TST/TT interfaces. This SLL structure induces a robust thermal confinement effect by utilizing the low thermal conductivity of the TT layers to block vertical heat dissipation, which significantly lowers switching energy and enhances cycling stability.

The resulting TST/TT SLL-based PCM device achieved a high-speed operation with a 15 ns pulse width and an ultra-low-power characteristic with a critical power density of 1.27 μW/nm. Notably, the SLL architecture yielded a 24.4% reduction in the phase-change threshold power compared to bulk TST devices, while simultaneously demonstrating exceptional endurance. These findings suggest that the TST/TT SLL architecture offers a viable and highly efficient pathway for the next generation of high-density data storage solutions.

---

**KEYWORDS:** Superlattice-like structure, Phase-change memory, Sputtering deposition, Doping, Storage-class memory

---

**ACKNOWLEDGEMENTS:** This research was supported by the Nano & Material Technology Development Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science and ICT (RS-2025-02217649).

---

### REFERENCES

- [1] H. Sung, J. Park, S. Kim, H. Song, C. Park, J. Park, S. Ju, and H. Lee, "Understanding the Effects of Ta Doping in Sb<sub>2</sub>Te<sub>3</sub> for High-Performance Phase Change Memory", *Adv. Eletron. Mater.* 11(8), 2400790 (2025).
- [2] H. Sung, J. Park, S. Kim, C. Park, J. Park, H. Lim, S. Lee, S. Park, and H. Lee, "Nanometer-Thick Films of Ta-doped Sb<sub>2</sub>Te<sub>3</sub>/TiTe<sub>2</sub> Superlattice-Like Nanostructures for Phase-Change Memory Data Storage", *ACS Appl. Nano Mater.* 9, 1453-1460 (2026).

## Ferroelectricity and hole transport property of organic semiconductors

T. Akutagawa<sup>1</sup>\*

1) Tohoku University, Japan

\* akutagawa AT tohoku.ac.jp

Benzo[b]benzo[4,5]thieno[2,3-d]thiophene (BTBT) derivatives are organic semiconductors known to exhibit high hole mobility due to the formation of two-dimensional electronic structures. In this presentation, we report on the phase transition behavior, molecular assembly structures, semiconductor properties, and ferroelectric properties of alkylamide-substituted organic ferroelectrics, R-BTBT-NHCOC<sub>14</sub>H<sub>29</sub> (**1**: R = H and **2**: R = C<sub>8</sub>H<sub>17</sub>). [1, 2]

The temperature- and frequency-dependent dielectric constants of **1** and **2** show the transition to SmE and SmC phases at 412 and 431 K, respectively, and melting at 468 and 479 K. The real part of the dielectric constant of **2** decreases monotonically with increasing temperature and shows a sharp frequency-dependent increase in dielectric constant from around 390 K. The dielectric constant of **1** is also affected by the temperature and frequency. This behavior is due to the activation of thermal motion of polar amide groups; both *P-E* curves of **1** and **2** show the hysteresis behavior of ferroelectrics near the solid-liquid crystal phase transition point, and the remanent polarization values and coercive electric field at 418 K and 0.1 Hz in **2** are 11.7 μC cm<sup>-2</sup> and  $E_c = 3.36$  V μm<sup>-1</sup>, respectively. Top-contact OFET devices were fabricated using the high-temperature deposited thin films **1** and **2**, and both showed p-type semiconducting output characteristics. The mobility of the deposited film **2** was  $1.01 \times 10^{-3}$  cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup>.

---

**KEYWORDS:** Ferroelectricity, Organic semiconductor, Hydrogen-bond, Dynamics

---

### REFERENCES

- [1] K. Sambe, T. Akutagawa, et al, ACS. Appl. Mater. Inter. 2023, 15, 58711.
- [2] K. Sambe, T. Akutagawa, et al, J. Am. Chem. Soc. 2024. 146, 8557.

## Ion energy effects on the formation of a 2D zirconium carbide during magnetron sputtering

M. Běloušek<sup>1, 1\*</sup>, M. Kormunda<sup>1</sup>, A. Jagerová<sup>1</sup>, M. Běloušek<sup>1</sup>

1) Jan Evangelista Purkyně University, Czech Republic

\* mbelous99 AT seznam.cz

2D transition metal carbides, nitrides and carbonitrides, so-called MXenes, gain increasing attention in materials science due to their exceptional physical properties. [1] Among them, zirconium carbide (ZrC) based MXenes are noteworthy for their predicted semiconducting behaviour. [2,3] Currently, the most common method of their preparation is acid etching. However, this approach limits the final morphology and size of prepared 2D flakes and thus their physical properties. [1,4] In contrast, physical vapor deposition (PVD) techniques offer improved control over the resulting chemical composition and morphology. [5] In this work, we investigate the effect of the energy delivered by ions formed in magnetron plasma on the amount of 2D ZrC phase formed at the C/Zr interface. The samples are prepared by magnetron deposition of ultrathin carbon layers (with maximal thickness of 2.5 nm) onto pre-deposited zirconium layers. By varying the working gas (Ar) pressure, the energy of ions was modified. The ion energy distributions (IEDs) analyzed with Hiden EQP 500 reveal, that the most energetic ions within the C target magnetron discharge are  $^{12}\text{C}^+$  ions, with mean energy 76.4 eV at a pressure 0.56 Pa. By depositing carbon onto the Zr surface,  $^{12}\text{C}^+$  ions carry enough energy to allow the formation of the ZrC phase at the C/Zr interface. With an increase in the pressure from 0.42 to 0.85 Pa, the  $^{12}\text{C}^+$  ions become more thermalized, leading to a decrease in their total delivered energy into the growing layer. This trend correlates with the XPS results, which indicate a reduction in the Zr-C bonding fraction (in at. %) with increasing pressure. Our findings explain the formation process of the ZrC phase at the C/Zr interface and further demonstrate that ion energy is a key parameter controlling the ZrC phase formation during magnetron sputtering.

**KEYWORDS:** MXenes, Magnetron sputtering, Zirconium carbide, Ion energy distribution function, XPS

**ACKNOWLEDGEMENTS:** The scientific results were obtained with the support of the University of J. E. Purkyně project UJEP-SGS-2025-53-003-3 and with the support of research infrastructure NanoEnviCz, supported by the Ministry of Education, Youth and Sports of the Czech Republic with project no. LM2023066.

### REFERENCES

- [1] X. Jiang, A.V. Kuklin, A. Baev, Y. Ge, H. Ågren, H. Zhang, P.N. Prasad, Two-dimensional MXenes: From morphological to optical, electric, and magnetic properties and applications. *Physics Reports*, 848 (2020), 1-58 (2020).
- [2] Y. Zhou, Z. Peng, Y. Chen, K. Luo, J. Zhang, S. Du, First-principles study of the electronic, optical and transport of few-layer semiconducting MXene. *Computational Materials Science*, 168 (2019), 137-143.
- [3] B. Ul Haq, S.H. Kim, R. Ahmed, K. Alam, A.M. Alsharari, A. Rasool Chaudhry, Investigations of Two-Dimensional Zirconium Carbide/Nitride MXenes in the Presence of Oxygen/Fluorine Functional Groups. *Journal of Solid State Chemistry*, 331 (2024), 124499.
- [4] S.A. Thomas, J. Cherusseri, Recent Advances in Synthesis and Properties of Zirconium-based MXenes for Application in Rechargeable Batteries. *Energy Storage*, 5 (2023), e475.
- [5] J. Vacík, P. Horák, S. Bakardjieva, V. Bejsovec, G. Ceccio, A. Cannavo, A. Torrìsi, V. Lavrentiev, R. Klie, Ion Sputtering for Preparation of Thin MAX and MXene Phases. *Radiation Effects and Defects in Solids*, 175 (2020), 177-189.

## Design of plastic crystalline materials via control of ionic and molecular motions through solid-solution formation

R. Tsunashima<sup>1\*</sup>

*1) Yamaguchi University, Japan*

\* ryotsuna AT yamaguchi-u.ac.jp

Solid solutions and alloys are widely used strategies for tuning the properties and functions of inorganic materials. According to the Hume-Rothery rule, atoms or ions with less than ~15% difference in size are generally miscible. While atomic sizes vary only moderately, material properties such as electronic configuration, spin state, and electronegativity can change significantly, enabling precise property control and even the emergence of new phases near composition boundaries.

In contrast, organic crystals exhibit much greater structural diversity, and their properties are governed by a delicate balance of molecular shape, intermolecular interactions, and electronic states. Although substitutions with halogens or heteroatoms may satisfy size-based miscibility criteria, they rarely induce substantial changes in physical properties. Furthermore, organic solid-solution formation typically relies on solution recrystallization, which imposes strict requirements on structural compatibility, such as lattice parameters and symmetry.

Despite these limitations, combining the structural diversity of organic molecules with solid-solution strategies offers a promising route to expand the accessible design space of molecular crystals. In particular, such approaches may enable exploration of multidimensional composition-structure-property relationships and uncover materials that fill the “gaps” in conventional molecular design.

In this presentation, we report new strategies for solid-solution design using structurally mismatched molecular pairs, which have comparable sizes but different symmetries. We demonstrate that such molecules become miscible when incorporated as molecular cations in ionic crystals.[1, 2] In addition, mechanochemical mixing provides an alternative route to achieve solid-solution formation.[3] These results highlight a new approach to overcoming shape constraints and open up new possibilities for the design and functional control of organic mixed crystals.

---

**KEYWORDS:** Solid solution, Ferroelectrics, Plastic crystals

---

### REFERENCES

- [1] Ryo Tsunashima et. al., *CrystEngComm.*, 2022, 24, 1309-1318 (Review).
- [2] Ryo Tsunashima et. al., *CrystEngComm*, 2020, 22, 2279.
- [3] Ryo Tsunashima et. al., *Chem. Commun.*, 2024, 60,12181.

## Formation of ultrathin and highly stable aromatic monolayers on silver surface—three legs are better than one

A. Rojek<sup>1\*</sup>, D. Cegiełka<sup>1</sup>, M. Wróbel<sup>1</sup>, M. Stępień<sup>1</sup>, Y. Shoji<sup>2</sup>, T. Fukushima<sup>2</sup>, M. Zharnikov<sup>3</sup>, P. Cyganik<sup>1</sup>

1) Smoluchowski Institute of Physics, Jagiellonian University, Poland

2) Institute of Integrated Research, Institute of Science Tokyo, Yokohama, Japan

3) Heidelberg University, Germany

\* anna.l.rojek AT uj.edu.pl

Surface functionalization using self-assembled monolayers (SAMs) is an effective strategy to tailor the morphology and electronic coupling of organic semiconductors (OSCs) at metal interfaces in organic electronic and photovoltaic devices. For optimal performance, such interlayers should be ultrathin, highly conductive, and composed of upright-oriented aromatic molecules, while also maintaining high thermal and chemical stability during OSC deposition and device operation [1-5]. In this work, we investigate the thinnest achievable aromatic SAMs on silver, a highly conductive electrode material. The studied systems are based on molecules with a thickness equivalent to a single phenyl ring and employ either conventional monodentate anchoring or triptycene-based, tridentate surface anchoring geometry.

A combination of surface-sensitive techniques, including X-ray photoelectron spectroscopy (XPS), infrared reflection-absorption spectroscopy (IRRAS), near-edge X-ray absorption fine structure (NEXAFS), and temperature-programmed desorption monitored by XPS, was used to comprehensively characterize the chemical composition, molecular orientation, bonding configuration, and thermal stability of the formed layers. Spectroscopic results confirm the formation of well-defined, upright, ultrathin (~0.8 nm) monolayers in both cases, with full engagement of anchoring groups, enabling a direct comparison of the two architectures.

Thermal desorption and chemical stability analyses reveal that monodentate systems exhibit lower stability, whereas triptycene-based tripods form significantly more robust monolayers. Notably, these ultrathin tridentate SAMs display stability comparable to, or exceeding, that of much thicker monodentate layers. This approach provides a promising pathway for interface engineering in organic electronics, with potential to enhance device performance.

**KEYWORDS:** Self-assembled monolayers, Triptycene, Thermal stability, Chemical stability, Spectroscopy

**ACKNOWLEDGEMENTS:** This study was funded by the National Science Centre, Poland (UMO-2022/47/B/ST5/01435) and partly supported by the Japan Society for the Promotion of Science (JSPS) (21H04690, 21H05024, and 20H05868 to T.F.) and the Cooperative Research Program of “Network Joint Research Center for Materials and Devices” from MEXT, Japan. The authors thank the Priority Research Area SciMat under the program Excellence Initiative—Research University at the Jagiellonian University in Kraków and the Materials Research Hub project for access to the Nano-Peak laboratory, where all XPS/TP-XPS measurements were conducted. M.Z. thanks the Helmholtz Zentrum Berlin (HZB) for allocating synchrotron radiation beamtime at BESSY II and for financial support. He also thanks Dr. M. Brzhezinskaya (HZB) for her assistance during the measurements at BESSY II.

### REFERENCES

- [1] M. Li, M. Liu, F. Qi, F.R. Lin, A.K.Y. Jen, Self-Assembled Monolayers for Interfacial Engineering in Solution-Processed Thin-Film Electronic Devices: Design, Fabrication, and Applications. *Chem. Rev.* 2024, 124 (5), 2138- 2204.
- [2] R. Gupta, J.A. Fereiro, A. Bayat, A. Pritam, M. Zharnikov, P.C. Mondal, Nanoscale Molecular Rectifiers. *Nat. Rev. Chem.* 2023, 7 (2), 106- 122.
- [3] M. Singh, N. Kaur, E. Comini, The Role of Self-Assembled Monolayers in Electronic Devices. *J. Mater. Chem. C* 2020, 8 (12), 3938- 3955.
- [4] S. Casalini, C.A. Bortolotti, F. Leonardi, F. Biscarini, Self-Assembled Monolayers in Organic Electronics. *Chem. Soc. Rev.* 2017, 46 (1), 40- 71.
- [5] A. Vilan, D. Aswal, D.L.A. Cahen, Ensemble Molecular Electronics: Motivation and Challenges. *Chem. Rev.* 2017, 117 (5), 4248- 4286.

## Dithiocarbamate-based self-assembled monolayers - the preparation method has a crucial impact on structure and stability

M. Wróbel<sup>1\*</sup>, M. Niemiec<sup>1</sup>, K. Kozieł<sup>2</sup>, P. Cyganik<sup>1</sup>

1) Smoluchowski Institute of Physics, Jagiellonian University, Poland

2) Faculty of Chemistry, Jagiellonian University, Poland

\* mat.wrobel AT uj.edu.pl

Dithiocarbamates (DTCs) are a promising class of molecules in which a bidentate anchoring group is used to functionalize metallic surfaces through the formation of self-assembled monolayers (SAMs). So far, two main strategies for the deposition of DTC SAMs have been employed interchangeably in the literature. In the first approach, the DTC compound is generated in situ via the condensation of a secondary amine with carbon disulfide directly in the presence of the metal substrate. In the second approach, a stable DTC salt precursor is synthesized beforehand and subsequently used to form monolayers from solution whenever required. Despite the extensive use of both methods, their direct comparison within a single experimental framework has been largely missing. Using the two model DTC SAMs based on phenylpiperidine and phenylpiperazine, we compared these two synthetic approaches for the first time in a single study [1]. We demonstrated that for the most crucial parameters of monolayers, such as packing density and thermal stability, there is a significant difference between the two formation methods, favoring the in situ method, which produces monolayers with high thermal stability (desorption energy  $\sim 1.5$  eV) and packing densities comparable to those of alkanethiols. On the other hand, we demonstrated that the overall chemical stability of DTCs is diminished compared to alkanethiols, which can be slightly improved using the in situ approach.

---

**KEYWORDS:** Dithiocarbamates, Self-assembled monolayers, Preparation technique, Thermal stability, Chemical stability

---

**ACKNOWLEDGEMENTS:** This work was funded by the National Science Center, Poland (UMO-2022/47/B/ST5/01435). The authors acknowledge support from the Priority Research Area SciMat under the Excellence Initiative - Research University programme at the Jagiellonian University in Kraków.

---

### REFERENCES

- [1] M. Wróbel, M. Niemiec, K. Kozieł, P. Cyganik, J. Phys. Chem. Lett. 16, 11526 (2025)

## Thermally stable aromatic SAMs for highly conductive or highly insulating organic monolayers on metals

P. Cyganik<sup>1</sup>\*

*1) Smoluchowski Institute of Physics, Jagiellonian University, Poland*

\* piotr.cyganik AT uj.edu.pl

Self-assembled monolayers (SAMs) on metal substrates are a key component of modern interfacial physical chemistry and advanced nanotechnology. The robustness of SAMs strongly depends on their thermal stability, which, together with electrical conductivity, constitutes a critical parameter for applications in molecular and organic electronics as well as photovoltaics.

In this work, we employ a multidisciplinary approach to investigate the structure, thermal stability, and conductivity of SAMs formed on metal substrates (Au or Ag) using various anchoring groups, including thiols, selenols, carboxylic acids, and carbenes.

Our recent results [1-5] demonstrate the formation of thin, well-defined monolayers exhibiting exceptionally high thermal stability. Depending on the molecular system, these SAMs can be either highly insulating or highly conductive, making them promising nanomaterials for the modification of gate or drain/source electrodes in organic field-effect transistors (OFETs).

---

**KEYWORDS:** Self-assembled monolayers, Organic electronics, Thermal stability, Conductivity

---

**ACKNOWLEDGEMENTS:** We acknowledge grants by National Science Centre Poland: UMO-2015/19/B/ST5/01636; DEC-2018/31/B/ST5/00057; UMO-2022/47/B/ST5/01435,

---

### REFERENCES

- [1] A. Krzykawska, M. Wróbel, K. Koziół, P.A.C.S. Cyganik, *Nano*, 14, 6043, (2020).
- [2] M. Wróbel, T. Żaba, E. Sauter, M. Krawiec, J. Sobczuk, A. Terfort, M. Zharnikov, and P. Cyganik, *Adv. Electron. Mater.*, 7, 2000947, (2021)
- [3] M. Wróbel, D. Cegiełka, A. Asyuda, K. Koziół, M. Zharnikov, P. Cyganik, *Nano Today*, 53, 102024, (2023).
- [4] A. Rojek, D. Cegiełka, M. Wróbel, Stępień, M.; Y. Shoji; T. Fukushima; M. Zharnikov; and Cyganik, P. *ACS Appl. Mater. Interfaces*, 18, 15665 (2026).
- [5] M. Wróbel, R. Ahmed, Bro-W. Jørgensen; K. Koziół; C.A. Nijhuis; G.C. Solomon; and Cyganik, P. under review 2026

## Surface-wettability interplay of thin films explored through photocatalysis

H. S<sup>1</sup>\*, D. K. G<sup>1</sup>

1) University of Kerala, India

\* heera AT keralauniversity.ac.in

Thin films are highly sensitive to surface properties due to the large proportion of atoms or molecules located at or near the surface. Consequently, surface characteristics such as roughness, surface energy, chemical functionality, and wettability play a crucial role in governing interfacial interactions and overall film performance. In this study, the surface properties of amorphous and crystalline Sb<sub>2</sub>S<sub>3</sub> thin films were systematically investigated, with particular emphasis on plasma-induced surface modification. Atomic force microscopy (AFM) revealed initial surface roughness values of 7.5 nm and 18 nm for the amorphous and crystalline films, respectively. Contact angle measurements indicated hydrophilic behavior for the amorphous film and slightly hydrophobic behavior for the crystalline film, with water contact angles of 68° and 92°, respectively [1,2]. Plasma treatment resulted in notable changes in surface morphology, including the formation of micro-/nanostructures and variation in surface roughness, as confirmed by AFM. The roughness increased to 14.4 nm for the amorphous film and slightly decreased to 17 nm for the crystalline film, contributing to changes in wettability [3]. The impact of these surface modifications was further demonstrated through photocatalytic activity studies using methylene blue degradation under visible light irradiation. The amorphous film exhibited superior photocatalytic performance, degrading 88% of the dye within 180 min with a reaction rate constant of 0.01 min<sup>-1</sup>, whereas the crystalline film achieved only 64% degradation under identical conditions. Following plasma treatment, the degradation efficiency decreased to 79% for the amorphous film and increased to 72% for the crystalline film, reflecting the influence of surface modifications on catalytic performance. These results clearly demonstrate the critical role of surface properties in determining the functional performance of Sb<sub>2</sub>S<sub>3</sub> thin films and highlight plasma treatment as an effective strategy for tailoring surface characteristics for application-specific optimization.

---

**KEYWORDS:** Thin film, Surface properties, Film roughness, Plasma treatment, Photocatalysis

---

**ACKNOWLEDGEMENTS:** The authors acknowledge funding through SARD, KSCSTE, Government of Kerala, India (003/2015/KSCSTE). Inspire Fellowship through DST, Government of India (IF200250) is also greatly acknowledged.

---

### REFERENCES

- [1] N. Nakazaki, H. Matsumoto, H. Tsuda, Y. Takao, K. Eriguchi, and K. Ono, “Surface smoothing during plasma etching of Si in Cl<sub>2</sub>,” *Applied Physics Letters*, vol. 109, no. 20, p. 204101, 2016, doi: 10.1063/1.4967474.
- [2] D. Y. Yun, W. S. Choi, Y. S. Park, and B. Hong, “Effect of H<sub>2</sub> and O<sub>2</sub> plasma etching treatment on the surface of diamond-like carbon thin film,” *Applied Surface Science*, vol. 254, no. 23, pp. 7925-7928, 2008, doi: 10.1016/j.apsusc.2008.03.170.
- [3] K. Guan, “Relationship between photocatalytic activity, hydrophilicity, and self-cleaning effect of TiO<sub>2</sub>/SiO<sub>2</sub> films,” *Surface and Coatings Technology*, vol. 191, nos. 2-3, pp. 155-160, 2005, doi: 10.1016/j.surfcoat.2004.02.022.

## Development of a method for producing self-fluxing nickel-based coatings by detonation spraying

N. Raisov<sup>1</sup>\*, D. Buitkenov<sup>1</sup>

1) Sarsen Amanzholov East Kazakhstan University, Ust-Kamenogorsk, Kazakhstan, Kazakhstan

\* nurmakhanbetraisov AT gmail.com

This study investigated the influence of detonation spraying process parameters on the structure and tribomechanical properties of self-fluxing coatings of the Ni-Cr-Fe-B-Si-C system. The variable parameters included the barrel fill volume (48-68%), the molar ratio of the working gases ( $O/C = 1.026-1.856$ ), and the delay time between shots (0-1 s). A morphological analysis of the coatings revealed the formation of a characteristic lamellar structure and the dependence of thickness and defects on spraying conditions. It was found that low barrel fill volumes result in a denser structure with minimal porosity, while medium and high barrel fill volumes result in the formation of microcracks due to increased residual stress. Tribological tests have shown that the minimum friction coefficient is achieved at a filling of 48% ( $\mu = 0.674 \pm 0.136$ ) and an O/C ratio of 1.026, but this also results in increased wear. The highest wear resistance is ensured at  $O/C = 1.856$  and an increased delay between shots (up to 1 s), at which the wear intensity decreases to  $0.000189 \text{ mm}^3/(\text{N}\cdot\text{m})$ . Roughness analysis showed that an increase in the delay between shots leads to a decrease in Ra from 5.00 to  $3.60 \mu\text{m}$ , which is associated with a decrease in the thermal load and improved conditions for coating formation. Maximum hardness (up to 905.6 HV) is achieved with an optimal combination of parameters, ensuring the formation of a dense structure and strengthening phases. It is shown that optimization of detonation spraying parameters requires a compromise between a decrease in the friction coefficient and an increase in wear resistance. The obtained results can be used in the development of technologies for the restoration and strengthening of machine parts.

**KEYWORDS:** Self-fluxing alloys, Detonation spraying, NiCrFeBSiC, Heat treatment, AISI 321

**ACKNOWLEDGEMENTS:** This research is funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. AP26103881).

### REFERENCES

- [1] S. Havrlisan, K. Simunovic, D. Vukelic, "Modelling of abrasive wear of Ni-based self-fluxing alloy coatings by the application of experimental design", *Technical Gazette*, 23, 1687-1693 (2006). <https://doi.org/10.17559/TV-20161020210442>.
- [2] K. Simunovic, T. Saric, G. Simunovic, "Different Approaches to the Investigation and Testing of the Ni Based Self-Fluxing Alloy Coatings-A Review", Part 1: General Facts, *Wear and Corrosion Investigations. Tribology Transactions*. 57, 255-279. (2014) DOI: 10.1080/10402004.2014.927547
- [3] S. Maksymova, V. Voronov, Kovalchuk P. "Brazing stainless steel with high chromium nickel alloy", *Research square*, (2025). <https://doi.org/10.21203/rs.3.rs-7259392/v1>
- [4] Tejero-Martin, D. Rezvani Rad, M. McA. Donald and T. Hussain "Beyond traditional coatings: A review on thermal-sprayed functional and smart coatings", *Journal of Thermal Spray Technology*, 28, 598-644 (2019). <https://doi.org/10.1007/s11666-019-00857-1>
- [5] D. Buitkenov, N. Raisov, T. Alimbekuly, B. Alibekova, "Study of the Tribological Properties of Self-Fluxing Nickel-Based Coatings Obtained by Gas-Flame Spraying", *Crystals*, 15(10), 862, (2025). <https://doi.org/10.3390/cryst15100862>. BR24992876

## Effect of dopant valence on infrared spectra of hafnia and zirconia films

D. Khomenkov<sup>1\*</sup>, L. Melnichuk<sup>1</sup>, O. Melnichuk<sup>1</sup>, F. Goubilleau<sup>2</sup>, D. Lehninger<sup>3</sup>, J. Heitmann<sup>4</sup>

1) Mykola Gogol State University of Nizhyn, 2 Hrafska str., Nizhyn 16600, Ukraine, Ukraine

2) CIMAP, CEA, UMR CNRS 6252, ENSICAEN, Normandie Université, 14000 Caen, France, France

3) Fraunhofer Institute for Photonic Systems, 01109 Dresden, Germany, Germany

4) Institute for Applied Physics, TU Bergakademie, Freiberg, Germany, Germany

\* dmkhomen AT gmail.com

Doped hafnia and zirconia are widely used as high-k materials in microelectronics, optics, and memory devices, where their functional properties are strongly influenced by defect structure and bonding configuration. Infrared (IR) spectroscopy provides a sensitive probe of these features; however, spectral interpretation remains challenging, especially for doped oxides due to the coexistence of different doping mechanisms.

In this work, the effect of dopant valence on FTIR spectra of HfO<sub>2</sub> and ZrO<sub>2</sub> films was studied. The films were grown on Si substrates by RF magnetron sputtering. Various dopants, namely, isovalent (Si, Ge), subvalent (Er, Nd), and supervalent (Ta), were introduced into the films during deposition, enabling controlled modification of defect structure and bonding.

The obtained results show that isovalent dopants (Si, Ge) do not introduce charge imbalance but lead to bond reconstruction and formation of mixed Me-O-Si or Me-O-Ge units (Me=Hf, Zr). As a result, IR spectra exhibit additional high-frequency absorption bands associated with Si-O (800-1100 cm<sup>-1</sup>) and Ge-O (600-900 cm<sup>-1</sup>) vibrations. At the same time, intrinsic Me-O phonon modes in the 250-700 cm<sup>-1</sup> region undergo a blue shift of ~10-30 cm<sup>-1</sup> (more pronounced for Si), remaining within the same spectral range while preserving their structure.

In contrast, subvalent dopants (Er, Nd) induce oxygen vacancies for charge compensation, leading to lattice distortion and reduced bond stiffness. This results in a characteristic red shift of vibrational modes by 10-40 cm<sup>-1</sup> (e.g., 500 → 470-490 cm<sup>-1</sup>), strong band broadening, and merging of spectral features, particularly in the monoclinic phase, as well as the appearance of weak defect-related bands in the 650-900 cm<sup>-1</sup> region.

Supervalent dopants (Ta) introduce excess electrons and modify IR spectra via electron-phonon interaction and screening effects. In this case, frequency shifts are relatively small (±5-10 cm<sup>-1</sup>), while the main changes include redistribution of band intensity, smoothing and asymmetry of spectral features, and moderate broadening. Additional high-temperature annealing (800-900 °C) further differentiates these mechanisms: strongly covalent Si-O bonds ensure high spectral stability, whereas vacancy-rich systems (Er, Nd) exhibit significant restructuring, and Ta-doped films vary mainly due to carrier redistribution. These mechanisms are discussed in detail. The results demonstrate that each dopant class produces a distinct spectroscopic fingerprint and provide a universal framework for interpreting IR spectra and assessing structural stability in HfO<sub>2</sub>- and ZrO<sub>2</sub>-based thin films. The obtained results are relevant for the development of high-k dielectrics, optical coatings, and resistive memory devices, where precise control of bonding, defect structure, and thermal stability is essential for device performance

---

**KEYWORDS:** HfO<sub>2</sub>, ZrO<sub>2</sub>, Infrared spectroscopy, Dopant valence, Thin films

## Posters

T5-16

E-POSTER

### The fabrication of multi-walled carbon nanotube thin films through laser-assisted growth techniques

I. S. Virt<sup>1</sup>\*, M. Chekailo<sup>2</sup>, A. Dziedzic<sup>3</sup>, S. Adamiak<sup>3</sup>, B. Cieniek<sup>3</sup>

1) Drohobych State Pedagogical University I. Franko, Ukraine

2) Department of Physics, Lviv Polytechnic National University, Lviv, Ukraine, Ukraine

3) Institute of Materials Engineering, University of Rzeszow, Rzeszow, Poland, Poland

\* isvirt AT email.ua

Multiwalled carbon nanotubes (MWNTs) are highly versatile nanostructures with broad industrial utility. This research investigates the application of pulsed laser deposition (PLD)-a technique noted for its ability to produce thin films with superior surface integrity and physical characteristics. Herein, MWNT films were synthesized by laser-ablating compressed targets (6–10 nm×2 μm) onto glass and Si(111) substrates. Comprehensive structural analysis via XRD and SEM verified film homogeneity and the presence of carbon-specific peaks. Furthermore, surface morphology was evaluated using Atomic Force Microscopy (AFM) to determine RMS roughness and fractal dimensions (DF). By utilizing the k-correlation (ABC) model to analyze Power Spectral Density (PSD) functions, the study characterizes the transition from primary grains to complex aggregates, revealing the fundamental growth mechanisms inherent in PLD-deposited MWNT films. This research explores the morphological dynamics of MWNT thin films fabricated through Pulsed Laser Deposition. By employing Power Spectral Density (PSD) analysis on AFM-derived data, we elucidate the correlation between laser fluence and grain clustering mechanisms. These findings offer a comprehensive understanding of the surface scaling and fractal topology inherent in laser-deposited carbon coating.

**KEYWORDS:** Multi-Walled carbon nanotubes (MWCNTs), Pulsed laser deposition (PLD), Atomic force microscopy (AFM), Surface topography

**ACKNOWLEDGEMENTS:** -

#### REFERENCES

- [1] A.K. Madikere Raghunatha Reddy, A. Darwiche, M.V. Reddy, K. Zaghib Review on Advancements in Carbon Nanotubes: Synthesis, Purification, and Multifaceted Applications, Batteries, 11(2), 71, (2025)
- [2] L.-M. Peng, Z. Zhang, S.g Wang Carbon nanotube electronics: recent advances, Materials Today, 17( 9), pp. 433-442 (2014).
- [3] L. Qian, Y. Xie, S. Zhang, J. Zhang Band Engineering of Carbon Nanotubes for Device Applications Matter, (3)3, pp. 664-695 (2020).
- [4] S. O. Abdellatif, Z. Khalifa Exploring the morphological surface resistance and optical absorption of thin black carbon nanotube films for electronic and optoelectronic devices 35, 623, (2024).

## Towards advanced wear-resistant coatings: Tailoring TiXN/NbN multilayers via alloying strategy

O. Maksakova<sup>1</sup>\*, V. Beresnev<sup>1</sup>, M. Sahul<sup>2</sup>, Z. Zhang<sup>3</sup>, S. Lytovchenko<sup>1</sup>

1) Education and Research Institute “School of Physics and Technology”, V.N. Karazin Kharkiv National University, Ukraine

2) Faculty of Materials Science and Technology, Slovak University of Technology in Bratislava, Slovakia

3) Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, Austria, Austria

\* o.maksakova AT karazin.ua

Multilayer nanolaminate coatings based on transition metal nitrides have attracted significant attention due to their ability to exhibit superior mechanical performance arising from interface-driven strengthening mechanisms [1]. In particular, Ti-based multilayers combined with NbN have demonstrated promising properties due to the synergistic interaction between constituent layers [2]. However, a systematic understanding of the role of alloying elements in Ti-based layers on the structural evolution and strengthening mechanisms of TiXN/NbN multilayers remains limited. In this work, a comparative study of TiXN/NbN (X = Zr, Si, Mo) multilayer coatings deposited by cathodic arc evaporation is presented. The influence of alloying element on phase composition, microstructure, and mechanical properties was investigated using advanced structural and mechanical characterization techniques.

The results reveal distinct growth mechanisms depending on the alloying element. TiZrN/NbN coatings exhibit a predominantly columnar structure with coherent growth across interfaces, indicating a strong template effect of NbN layers. In contrast, TiSiN/NbN multilayers demonstrate the formation of amorphous TiSiN nanolayers, which disrupt epitaxial growth and lead to a featureless morphology. TiMoN/NbN coatings show refined microstructure and enhanced tribological performance, associated with solid solution strengthening and grain refinement effects. Despite comparable hardness values, the coatings exhibit fundamentally different strengthening mechanisms governed by the nature of the alloying element. The obtained results highlight that the selection of alloying component in Ti-based layers provides an effective pathway for tailoring microstructure and optimizing mechanical performance of multilayer coatings. This study provides new insights into the design of advanced multilayer coatings with controlled architecture and enhanced functional properties for industrial applications.

---

**KEYWORDS:** Protective coatings, TMNs, Alloying, Hardness, Wear-resistance

---

**ACKNOWLEDGEMENTS:** This work is supported by the Ministry of Education and Science of Ukraine (MES) under the National Budget Program (Project 0124U001127).

---

### REFERENCES

- [1] O. Maksakova, S. Lytovchenko, V. Beresnev, S. Klymenko, D. Horokh, B. Mazilin, M. Kopeykina, S. Klymenko, V. Grudnitski, O. Gluhov, and R. Galushkov. “A Review of Vacuum-ARC Multilayer Coatings with High-Strength Characteristics and Adhesive Properties”, *East Eur. J. Phys.*, 4, 11-24 (2024).
- [2] W. Cheng, J. Wang, X. Ma, P. Liu, P.K. Liaw, and W. Li, “A review on microstructures and mechanical properties of protective nano-multilayered films or coatings”, *J. Mater. Res. Technol.*, 27, 2413-2442, (2023).

## Electrical conductivity of thin films of CoNi, FeNi, and CuNi alloys

V. B. Loboda<sup>1</sup>, S. Khursenko<sup>1\*</sup>, V. Kravchenko<sup>1</sup>, O. Yurchenko<sup>1</sup>

*1) Sumy National Agrarian University, Ukraine*

\* khursenkosvetlana AT gmail.com

This paper presents the results of a study of the electrical conductivity of structurally continuous nanocrystalline films of CoNi, FeNi, and CuNi alloys in the thickness range of 10-200 nm and a wide range of component concentrations. CoNi and FeNi alloy films were obtained by condensation of evaporated initial bulk binary CoNi and FeNi alloys, while CuNi alloy films were obtained by simultaneous, separate evaporation of the components (copper and nickel) in a vacuum of  $10^{-4}$  Pa. Nickel and bulk alloys were evaporated using an electron beam evaporation method using an electron diode gun. Copper was evaporated from a 0.05 mm thick tungsten foil ribbon. The condensation rate was 0.5-1.5 nm/s. Thermal stabilization of the electrical properties of the alloy films was achieved through three heating-cooling cycles in the temperature range of 300-700 K. The dependences of the film electrical resistance on the annealing temperature were studied. For all alloy films, the temperature dependence curves of electrical resistance for the second and subsequent heating-cooling cycles were virtually identical, indicating complete stabilization of the electrical properties of the film samples after the second annealing cycle. A specific irreversible decrease in the electrical resistance of the films after heat treatment was experimentally revealed, indicating ordering of the film structure. It was shown that the nature of the change in electrical resistance depends on both the thickness of the alloy films and the ratio of the alloy components. To explain the observed decrease in electrical resistance during thermal stabilization of the electrical properties of the films of the studied alloys, we used the Wend model, which describes the healing of defects in the crystalline structure of the films and the improvement of structural ordering. Based on this model, crystal structure defect spectra were calculated in films of the studied CoNi, FeNi, and CuNi alloys.

---

**KEYWORDS:** Thin films, Nanocrystalline films, Electrical conductivity, Crystal structure defects, Activation energy for defect healing

## Contact mechanics of Pb, Cu, and Al nanoparticles

A. Samilyk<sup>1</sup>, M. Prodanov<sup>1\*</sup>, A. V. Khomenko<sup>1</sup>

1) Sumy State University, Ukraine

\* prodanov.my AT gmail.com

Tribological properties of metal nanoparticles (NPs) adsorbed on various surfaces can be unique. Experimentally and numerically, it has been shown that copper, gold, silver, and antimony NPs adsorbed on various substrates can exhibit superlubricity [1], frictional anisotropy [2], and a significant dependence of the friction force on the environmental conditions [3]. Fundamentally, it is expected that a quantitative understanding of the atomistic origins of friction will enable the explanation of well-known macroscopic tribological laws. From a practical point of view, this will facilitate control of adhesion, friction, and wear at the nanometer scale, which is important for the rapidly developing applications of metallic NPs in medicine, pharmaceuticals, cosmetics, catalysts, batteries, sensors for the detection of toxic heavy metals, etc.

In general, the quantitative characterization of tribological properties is based on the concepts of contact mechanics (CM), such as the apparent, absolute, and relative contact areas of surfaces, the average distance between them, the distribution of interfacial distances and forces, topography, in particular, the power spectrum of surface roughness, and root-mean-square roughness [4]. However, unlike the existing knowledge of thermodynamic, optical, and other properties, there is no literature data on the size scaling of CM properties of NPs.

In this work, we investigate the size scaling of the CM properties of Cu, Al, and Pb NPs adsorbed on a suspended graphene substrate using classical molecular dynamics simulations. The large-scale model enabled us to consider NPs with diameters ranging from 1 nm to approximately 50 nm. The simulations suggest that the NPs' contact surfaces are not flat, which is confirmed by the height distributions of the contact surface of NPs that can roughly be subdivided into three parts: a narrow Gaussian spike, the uniform height section, and a Gaussian tail. The surface height can vary by more than 1 nm. In contrast, the distribution of the distances between the surfaces can be approximated by a single Gaussian. The variation in the interfacial gap is only a few Å. The isotropic height power spectral density (PSD) of the contact surface of NPs larger than about 20 nm in diameter exhibits relatively narrow power-law regions. Our simulations suggest that NPs formed on a macroscopically smooth graphene can exhibit random roughness. The results provide a basis for the quantitative description of NP contact mechanics by estimating PSDs that can be used in analytical theories for atomistic systems.

---

**KEYWORDS:** Contact mechanics, Graphene, Molecular dynamics, Topography

---

### REFERENCES

- [1] E. Cihan, D. Dietzel, B. R. Jany and A. Schirmeisen, “Effect of amorphous-crystalline phase transition on superlubric sliding”, *Phys. Rev. Lett.*, 130, 126205 (2023).
- [2] O.V. Khomenko, A.A. Biesiedina, K.P. Khomenko, P.E. Trofimenko, and I.A. Chelnokov, “Atomistic modelling of frictional anisotropy of metal nanoparticles on graphene”, *Progress in Physics of Metals*, 26, 219-254 (2025).
- [3] W. H. Oo, H. Gao, M. H. Müser and M. Z. Baykara, “Persistence of structural lubricity on contaminated graphite: rejuvenation, aging, and friction switches”, *Nano Letters*, 24, 12118-12124 (2024).
- [4] N. Rodriguez, L. Gontard, C. Ma, R. Xu and B. N. J. Persson, “On how to determine surface roughness power spectra” *Tribol. Lett.*, 73, 18 (2025).

## DEvelopment of bifunctional polymer surfaces via fs laser structuring and subsequent chitosan/Cu deposition

A. Daskalova<sup>1\*</sup>, L. Angelova<sup>1</sup>, I. Ercerg<sup>2</sup>, T. Car<sup>2</sup>, M. Sikiric<sup>2</sup>

1) Institute of Electronics, Bulgarian Academy of Sciences, Bulgaria

2) Rudjer Boskovic Institute RBI, Croatia

\* albdaskalova AT gmail.com

One of the most widely used biomaterials in tissue engineering field is the polylactic acid (PLA). Due to its easily customizable properties the scaffolds made from PLA support effectively tissue regeneration. Despite effective PLA biodegradability and biocompatibility characteristics, the polymer lacks antimicrobial activity, which raises the need to further modification of its surface performance for applications in tissue engineering [1,2] In this research, poly lactic acid (PLA) matrices were textured via femtosecond laser processing using a galvanoscanner module. The designed structures exhibited micron sized hierarchical hydrophobic surface structures. Ultra-short laser modification is a non-contact method for modification of a variety of materials. It proceeds with creation of defined, precise with minimal thermal damage processing zones, allowing the creation of well-defined surface structures that affects surface wettability state, surface energy, and subsequently cell-material interactions [3]. The obtained laser textures provide hydrophobic surface behavior, due to formed hierarchical structures which promotes a Cassie-Baxter wetting regime. Additional functionalization of structured PLA by spin coating deposition of a chitosan layer was performed, which altered the wettability states by minimizing the water contact angle after laser processing. The different wetting behaviors of the structures before and after chitosan layer deposition were correlated with the surface structures and wetting states. Comprehensive characterizations of the surface characteristics surface roughness, and wetting dynamics of different textures before and after chitosan layer deposition were done for comparative investigation. In parallel, magnetron sputtered copper (Cu) was deposited onto the femtosecond laser structured PLA matrices, in order to introduce additional antimicrobial functionality. This step additionally provides factors such as Cu loading, distribution, oxidation state, or release kinetics may contribute to overall antimicrobial performance of the designed matrix. The current study provides a method to combine fs laser structuring with additional functionalization with biopolymer and separately a comparison with metallic thin layer, for obtaining a comparative results in the case of multifunctional surface engineering. However, optimization of the metallic deposition parameters is necessary to achieve effective antimicrobial activity. These findings contribute to the development of advanced biofunctional surfaces for biomedical applications.

---

**KEYWORDS:** Biomaterials, Femtosecond laser modification, Tissue engineering, Functionalization

---

**ACKNOWLEDGEMENTS:** This research was funded by the BULGARIAN NATIONAL SCIENCE FUND (NSF) under Project No. KP-06-H98/1, (2025-2028), and partly under grant number KP-06-Austria/5 (2025-2027).

---

### REFERENCES

- [1] B. Kryszaka, K. Szustakiewicz, P. Dzienny, Adam Junka, Justyna Paleczny, Patrycja Szymczyk-Ziołkowska, Viktoria Hoppe, Arkadiusz Antonczak, Functionalization of the PLLA surface with a femtosecond laser: Tailored substrate properties for cellular response, *Polymer Testing* 116 (2022) 10781
- [2] Z. Brounstein, M. Chris. Yeager and Andrea Labouriau, Development of Antimicrobial PLA Composites for Fused Filament Fabrication, *Polymers* 2021, 13(4), 580; <https://doi.org/10.3390/polym13040580>
- [3] K. Schwibbert, M. Anja. Richter, Jörg Krüger, and Jörn Bonse, Textured Surfaces: A Way to Control Biofilm Formation? , *Laser Photonics Rev.* 2024, 18, 2300753

## Preparation of TiO<sub>2</sub>-Cr<sub>2</sub>O<sub>3</sub> composite powder based on nanoparticles using spray drying for atmospheric plasma spraying

D. Kakimzhanov<sup>1,2\*</sup>, B. Rakhadilov<sup>3</sup>, Z. Satbayeva<sup>3</sup>

1) D. Serikbaev East Kazakhstan Technical University, Kazakhstan

2) Shakarim State University of Semey, Kazakhstan

3) Shakarim University, Kazakhstan

\* d.kakimzhanov19 AT gmail.com

In this study, composite coatings based on TiO<sub>2</sub> and TiO<sub>2</sub>-Cr<sub>2</sub>O<sub>3</sub> nanopowders were produced by atmospheric plasma spraying for use in high-temperature acid leaching conditions. The initial nanopowders were first agglomerated in an aqueous medium with the addition of polyvinyl alcohol, after which spherical granules were formed from them by spray drying. The coatings were applied to substrates made of corrosion-resistant steel 12Kh18N10T. According to X-ray diffraction analysis, the main crystalline components of the coatings were rutile TiO<sub>2</sub> and Cr<sub>2</sub>O<sub>3</sub>, with a small amount of Ti<sub>2</sub>O<sub>3</sub> present. In coatings formed solely from TiO<sub>2</sub>, the rutile phase predominated, whilst anatase was detected in insignificant quantities and brookite was not observed. The predominance of rutile is due to the high-temperature conditions of plasma spraying, which promote the phase transformation of anatase into the more stable rutile modification. The coatings obtained were characterised by a dense structure and low porosity, which is attributed to the optimisation of both the preparation of the powder material and the spraying conditions. The introduction of Cr<sub>2</sub>O<sub>3</sub> resulted in a significant increase in the microhardness of the coating to 1015 HV, whereas for the pure TiO<sub>2</sub>-based coating this figure was 723 HV.

**KEYWORDS:** Coatings, Plasma spraying, Wear resistance, Spray dryer

**ACKNOWLEDGEMENTS:** This research has been funded by the Committee of Science of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. BR24992870)

### REFERENCES

- [1] L. Vernhes, M. Azzi, E. Bousser, T. Schmitt, J.M. Lamarre, Klemberg-Sapieha, J.E.: Hybrid Co-Cr/W-WC and Ni-W-Cr-B/W-WC Coating Systems. *J Therm Spray Tech.* 25, 346-356 (2016). <https://doi.org/10.1007/s11666-015-0357-5>
- [2] M. Pearson, F. Cheuk, C. Sist, : An Entropy Approach to Optimizing Heat Recovery in High-Pressure Autoclave Circuits. In: *Proceedings of the 62nd Conference of Metallurgists, COM 2023.* pp. 79-97. Springer Nature Switzerland, Cham (2023)
- [3] J. Vaughan, P. Reid, A. Alfantazi, : Corrosion of Ti-2 and Ti-7 relevant to nickel acid leach chemistry. *Hydrometallurgy.* 101, 156-165 (2010). <https://doi.org/10.1016/j.hydromet.2009.12.011>
- [4] G.E. Kim, T.A. Brzezinski, L. Leblanc, E. Kharlanova, Thermal spray coatings for ball valves used in Nickel/Cobalt pressure acid leaching. In *International Thermal Spray Conference.* - ASM International 2000, 83607, 1149-1153
- [5] B.K. Rakhadilov, D.B. Buytkenov, D. Kakimzhanov, R.S. Kozhanova, G.S. Bektasova, The effect of detonation spraying on the phase composition and hardness of Al<sub>2</sub>O<sub>3</sub> coatings. *Eurasian Journal of Physics and Functional Materials*, 4(2), 160-166 (2020).

## Ferroelectric-like double P-E hysteresis of plastic crystalline succinonitrile based on rotational and conformational degrees of freedom

N. Onodera<sup>1</sup>\*, S. Dekura<sup>2</sup>, T. Sato<sup>2</sup>, T. Akutagawa<sup>2</sup>

1) Graduate School of Engineering, Tohoku University, Japan

2) Tohoku University, Japan

\* onodera.nozomi.s5 AT dc.tohoku.ac.jp

Organic molecular solid materials often exhibit intermediate phases between solid and liquid states, such as liquid crystal (LC) and plastic crystal (PC) phases, due to the balance of relatively weak intermolecular interactions (e.g., van der Waals and hydrogen bonding interactions). In particular, PC materials, which have the ordered molecular center of gravity with the disordered molecular orientation, i.e. rotational dynamics, are promising candidates for next-generation memory materials due to their dynamic nature [1]. In this study, we focused on succinonitrile (SN), which exhibits a PC phase between 233 and 328 K. In addition to the rotational degree of freedom, SN possesses conformational degree of freedom; SN exhibits two stable conformations with distinct electric dipole moments, gauche and trans conformations, in the PC phase [2]. Because of these peculiar two degrees of freedom, it is expected that SN can show unconventional dielectric properties. However, the dielectric properties of SN remained largely unexplored. Here we show that SN forms a unique polarized orientation state in the PC phase [3]. We discovered that SN exhibits hysteresis in the polarization-electric field (*P-E*) curves in the PC phase above 240 K. Notably, such *P-E* hysteresis curve has not been observed in the PC phase of previously reported ionic plastic crystals although they show ferroelectricity in the low-temperature crystalline phase [1,4]. To the best of our knowledge, this is the first example of ferroelectric-like *P-E* hysteresis in a PC phase. Furthermore, current-electric field (*J-E*) curves (the first derivative of the *P-E* curves) revealed two distinct current peaks corresponding to polarization reversal. This result suggests the existence of two different polarization mechanisms of SN, originating from the molecular orientational and conformational degrees of freedom. The discovery of *P-E* hysteresis in the PC phase represents a significant leap toward unlocking the latent potential of the PC materials. Moreover, the existence of two different polarization reversal mechanisms is expected to be a key to realizing high-density memory that can use quaternary states, thereby surpassing conventional memories using binary states.

**KEYWORDS:** Succinonitrile, Plastic crystal, Molecular dynamics, Ferroelectricity

**ACKNOWLEDGEMENTS:** This work was supported by a Grant-in-Aid for Scientific Research on KAKENHI (Grant Numbers: JP20H05865 and 23K13715), Japan Science and Technology Agency, ACT-X (Grant Number: JPMJAX23DF), the "Crossover Alliance to Create the Future with People, Intelligence and Material" project supported by the Ministry of Education, Culture, Sports, Science, and Technology, and research grants from Yamada Science Foundation and Amano Institute for Technology.

### REFERENCES

- [1] J. Harada, T. Shimojo, H. Oyamaguchi, H. Hasegawa, Y. Takahashi, K. Satomi, Y. Suzuki, J. Kawamata, T. Inabe, "Directionally Tunable and Mechanically Deformable Ferroelectric Crystals from Rotating Polar Globular Ionic Molecules." *Nat. Chem.* 2016, 8, 946-952.
- [2] O.I. Fengler, A. Ruoff, "Vibrational spectra of succinonitrile and its [1,4-13C<sub>2</sub>]-, [2,2,3,3-2H<sub>4</sub>]- and [1,4-13C<sub>2</sub>-2,2,3,3-2H<sub>4</sub>]-isotopomers and a force field of succinonitrile." *Spectrochim. Acta A* 2001, 57, 105-117.
- [3] N. Onodera, S. Dekura, T. Sato, M. Mashiko, T. Kurihara, M. Mizuno, T. Akutagawa, "Ferroelectric-like Polarization Switching in Plastic Crystalline Succinonitrile." *J. Am. Chem. Soc.* 2025, 147, 19200-19209.
- [4] J. Harada, Y. Kawamura, Y. Takahashi, Y. Uemura, T. Hasegawa, H. Taniguchi, K. Maruyama, "Plastic/Ferroelectric Crystals with Easily Switchable Polarization: Low-Voltage Operation, Unprecedentedly High Pyroelectric Performance, and Large Piezoelectric Effect in Polycrystalline Forms." *J. Am. Chem. Soc.* 2019, 141, 9349-9357.

## Influence of acid modification on the protective properties of montmorillonite nanoreservoirs as anticorrosion pigment

M. Danyliak<sup>1</sup>\*, S. Korniy<sup>1</sup>

*1) Karpenko Physico-Mechanical Institute of the National Academy of Sciences of Ukraine, Ukraine*

\* danyliak-olena AT ukr.net

Polymer coatings are widely used to protect aluminium alloys from corrosion [1]. Their long-term effectiveness is due to the presence of anti-corrosion pigments such as chromates. However, chromate pigments are carcinogenic and toxic. A more environmentally friendly alternative to chromates is pigments based on natural minerals, such as aluminosilicates. In particular, aluminosilicate minerals such as montmorillonite have a layered nanostructure and can be used as nanoreservoirs loaded with an anticorrosion inhibitor [2]. The modification of montmorillonite with organic acids improves its protective anti-corrosion properties, making it a promising anti-corrosion pigment.

Therefore, the aim of the work was to obtain eco-friendly anti-corrosion pigment based on montmorillonite nanoreservoirs modified with  $\text{CH}_3\text{C}(\text{OH})(\text{H}_2\text{PO}_3)_2$  acid and to evaluate their inhibitory efficiency for an AA<sub>2024</sub> aluminium alloy in an acid rain environment with pH = 4.5.

The anticorrosion pigment based on the montmorillonite nanoreservoirs acid modified was obtained by liquid phase ion exchange. Montmorillonite from bentonite was purgated by the coarse-dispersed phase sedimentation method [3]. The montmorillonite nanoreservoirs acid modified increases the corrosion resistance of the an AA<sub>2024</sub> aluminium alloy in the acid rain environment. According electrochemical impedance spectroscopy results, it was established that the value of charge transfer resistance ( $R_{ct}$ ) of the aluminium alloy was  $3.4 \cdot 10^4 \Omega \times \text{cm}^2$ , after 24 hours of immersion in the acid rain environment. The addition of acid modified montmorillonite to the environment causes a gradual release of phosphonate anions, adsorbed on the alloy surface through complexation with metal ions. The value of  $R_{ct}$  of the aluminium alloy was  $8.4 \cdot 10^4 \Omega \times \text{cm}^2$ , after 24 hours of immersion in an inhibited environment.

Thus, acid modification of montmorillonite nanoreservoirs is effectively for corrosion protection of aluminium alloy in an acid rain environment.

---

**KEYWORDS:** Montmorillonite, Acid modification, Corrosion, Nanoreservoirs, Polymer coatings

---

**ACKNOWLEDGEMENTS:** The work was performed within the project No. 2025.07/0048 “Development of new environmentally friendly inhibitory compositions for protection against tribocorrosion and corrosion fatigue of aluminum alloy structures” of the National Research Foundation of Ukraine.

---

### REFERENCES

- [1] S. Korniy, M.-O. Danyliak, and I. Zin, “Zeolite-based anti-corrosion pigments for polymer coatings: a brief review,” *Adv. Polym. Technol.*, 2024, 6533170 (2024).
- [2] M.O.M. Danyliak, and S.A. Korniy, “Inhibitory properties of an ion-exchange anti-corrosion pigment based on the natural montmorillonite for paint coatings,” *Mater. Sci.*, 60, 335-343 (2024).
- [3] V. V. Kochubei, Ya. V. Yaremchuk, S. G. Yabolnyk, and M.-O. Danyliak, “Sorption capacity of ultrasound-activated natural bentonite regarding copper ions,” *Mater. Sci.*, 60, 97-103 (2024).

## N-alkyl xanthic acids monolayers on metal substrates: Structure and bonding

M. Szatny<sup>1</sup>\*, M. Lebica<sup>1</sup>, M. Wróbel<sup>1</sup>, D. Cegielka<sup>1</sup>, P. Cyganik<sup>1</sup>

*1) Smoluchowski Institute of Physics, Jagiellonian University, Poland*

\* marta.szatny AT student.uj.edu.pl

The development of nanotechnology is increasingly based on combining organic and inorganic materials, where the interface between them plays an important role in determining the properties and performance of the system. Self-assembled monolayers (SAMs) are one of the main methods used to control the structure and physicochemical properties of such metal-organic interfaces [1,2]. The most studied system is based on alkanethiols on Au(111), in which molecules attach to the surface through a single sulphur atom [3]. In addition, bidentate systems such as n-alkyl xanthogenates can form densely packed and well-ordered SAMs on Au(111), providing an alternative binding mode involving two sulphur atoms [4].

In this work, n-alkyl xanthogenate SAMs ( $-\text{S}_2\text{CO}-(\text{CH}_2)_n-\text{CH}_3$ ) formed on Au(111) and Ag(111) substrates were studied, with a focus on the effect of the solvent on the structure and stability of the monolayers. The formation process and structural quality were analysed using infrared reflection-absorption spectroscopy (IRRAS), X-ray photoelectron spectroscopy (XPS), and water contact-angle (CA) measurements. The results show that ethanol, isopropanol, and dichloromethane lead to well-ordered and densely packed layers on both substrates. Meanwhile, on gold, good-quality monolayers can also be obtained using water.

Although the overall structural ordering is similar, the bonding between the molecules and the surface is different for the two metals. On Au(111), xanthogenate molecules predominantly bind via both sulfur atoms. In contrast, on Ag(111), monolayer formation may involve modification of xanthogenate group into thioester. In these configuration only one sulfur atom binds molecule to the metal surface, while the other dissociates from the molecule and binds directly to the substrate. The unsaturated carbon atom from xanthogenate group forms carbonyl group with additional oxygen atom. This interpretation is supported by the observed correlation between the carbonyl-related signal and chemisorbed sulfur.

These results show that both the type of metal substrate and the preparation conditions have a strong influence on the structure, bonding, and stability of xanthogenate SAMs, which is important for designing functional organic-inorganic interfaces.

---

**KEYWORDS:** Self-assembled monolayers (SAMs), Xanthogenates, Metal surfaces, XPS, IRRAS

---

**ACKNOWLEDGEMENTS:** This work was funded by the National Science Center, Poland (OPUS-2022/47/B/ST5/01435).

---

### REFERENCES

- [1] A. Ulman, "Formation and Structure of Self-Assembled Monolayers", *Chem. Rev.*, 96, 1533-1554 (1996).
- [2] J. C. Love, L. A. Estroff, J. K. Kriebel, R. G. Nuzzo, and G. M. Whitesides, "Self-Assembled Monolayers of Thiolates on Metals as a Form of Nanotechnology", *Chem. Rev.*, 105, 1103-1169 (2005).
- [3] C. Vericat, M. E. Vela, G. Benitez, P. Carro, and R. C. Salvarezza, "Self-Assembled Monolayers of Thiols and Dithiols on Gold: New Challenges for a Well-Known System", *Chem. Soc. Rev.*, 39, 1805-1834 (2010).
- [4] H. J. Moore, R. Colorado, H. J. Lee, A. C. Jamison, and T. R. Lee, "Synthesis, Characterization, and Relative Stabilities of Self-Assembled Monolayers on Gold Generated from Bidentate n-Alkyl Xanthic Acids", *Langmuir*, 29, 10674-10683 (2013).

## Image segmentation-based quantitative analysis of surface topography in HfZrTiTaNb-cx coatings

D. Kondrakhova<sup>1\*</sup>, P. Hviščová<sup>1</sup>, L. Kvetková<sup>1</sup>, Y. Rozghon<sup>2</sup>, V. Kharchenko<sup>2,3</sup>, A. Dvornichenko<sup>2</sup>, F. Lofaj<sup>1</sup>

1) Institute of Materials Research, Slovak Academy of Sciences, Košice, Slovakia

2) Sumy State University, Ukraine

3) Institute of Applied Physics, National Academy of Sciences of Ukraine, Ukraine

\* dkondrakhova AT sasko.sk

High-entropy ceramics (HECs) are multicomponent solid solutions containing four or more main elements at near-equiatomic concentrations [1]. These materials offer an alternative to the classical development approach, which has been successfully adapted from metallic alloys to ceramic systems. Of particular interest are high-entropy carbides based on Group IV-V metals, which demonstrate high hardness, wear resistance and resistance to extreme operating conditions [2,3]. Their unique properties are due to a combination of strong covalent bonds and pronounced lattice distortion effects arising from their multicomponent composition [4].

In this study, high-entropy HfZrTiTaNb-Cx coatings were deposited by DC magnetron co-sputtering from two independent sources. The carbon content was varied by adjusting the power of the carbon target within the range of 200-600 W. The effect of carbon on the structural and morphological properties was comprehensively investigated using X-ray diffraction (XRD), atomic force microscopy (AFM) and Raman spectroscopy. Surface topography was analysed by image segmentation followed by statistical and morphological analysis of the identified structures.

The results of a quantitative analysis of AFM images show that surface morphology is strongly dependent on carbon content. With increasing carbon content, surface roughness increases and the structure exhibits a non-monotonic evolution, accompanied by the coarsening of nanostructures at high power levels. This behavior may be associated with their coalescence and the formation of a carbon phase at elevated carbon contents.

Raman spectroscopy confirmed the formation of an amorphous sp<sup>2</sup>-bonded carbon phase at high carbon content, indicating a transition from a single-phase carbide system to a two-phase structure (carbide + graphite-like carbon). XRD confirms a single-phase fcc carbide (Fm-3m) with lattice expansion at higher carbon content. All samples exhibit a predominant (111) texture, characteristic of transition metal carbides.

The obtained results demonstrate the key role of carbon content in determining the properties of HfZrTiTaNb-Cx coatings and confirm their potential for further research into the relationship between structure, morphology and mechanical characteristics.

---

**KEYWORDS:** High-entropy carbides, Magnetron co-sputtering, Carbon content, Dual-phase structure, Surface morphology

---

**ACKNOWLEDGEMENTS:** This work was supported by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under project No. 09I03-03-V04-00281 and by the Slovak Research and Development Agency (project APVV-24-0038) and VEGA 2/0115/26.

---

### REFERENCES

- [1] J.M. Schneider, 'How high is the entropy in high entropy ceramics?' *J. Appl. Phys.*, 130(15), 150903. <https://doi.org/10.1063/5.0062523> (2021).
- [2] aková, L., M. Hrubovčáková, A. Kovalčíková, D. Medved', *et al.* (2024). 'Influence of sintering condition on tribological properties of (Hf-Ta-Zr-Nb-Ti)C carbides'. *Int. J. Refract. Met. Hard Mater.*, 119, 106549. <https://doi.org/10.1016/j.ijrmhm.2023.106549>
- [3] Y. Fan, Y. Chen, J. Wang, L. Gu, *et al.* (2026). 'Insights into crystal growth and morphology evolution mechanism of multi-component carbide: Experiments and first-principles calculations'. *J. Mater. Sci. Technol.*, 240, 27-34. <https://doi.org/10.1016/j.jmst.2025.03.057>
- [4] W.W. Sun, *et al.*, 'Influence of metal element types on the density, phase purity, and mechanical properties of high-entropy carbide ceramics'. *Int. J. Refract. Met. Hard Mater.*, 136 (2026), 107578. <https://doi.org/10.1016/j.ijrmhm.2025.107578>

## Polymer membranes based on polyelectrolyte complexes

V. Demchenko<sup>1</sup>\*

1) *E.O. Paton Electric Welding Institute of the National Academy of Sciences of Ukraine, Ukraine*

\* dvaleriy1 AT ukr.net

In the modern world, the problem of ensuring access to quality water remains acute. This is due to global challenges such as the growth of industrial production, population growth, climate change, and the reduction of fresh water reserves. Water purification membranes, as a key technology in the field of water purification and reuse, require modernization of production to meet growing needs.

The most common contaminants found in water are heavy metals, synthetic dyes and petrochemical residues. In addition, in recent years, attention has been increasing to micropollutants, in particular pharmaceuticals and personal care products, which is associated with increased awareness of their impact on the environment, public health and the economy.

The structure, thermal, thermomechanical and sorption properties of polyelectrolyte complexes (PECs) pectin-chitosan, pectin-cationic starch and CMC-cationic  $\beta$ -CD were investigated. Using the IR spectroscopy method, it was found that the spectra of all studied polyelectrolyte complexes contain two intense bands in the region of  $1417-1423\text{ cm}^{-1}$  and  $1616-1623\text{ cm}^{-1}$ , which can be attributed to symmetric and asymmetric deformation vibrations of ionized carboxyl groups, which confirms the formation of polyelectrolyte complexes. Analysis of wide-angle X-ray diffraction patterns of the studied samples showed that pectin and Na-CMC are characterized by an amorphous structure, while cationic starch, chitosan and  $\beta$ -CD have a semi-crystalline structure. The highest degree of crystallinity is characteristic of PECs pectin-cationic starch and is 75%. It was found that the best thermal and thermomechanical indicators are possessed by the polymer system CMC-cationic  $\beta$ -CD (destruction onset temperature  $274\text{ }^{\circ}\text{C}$ , glass transition temperature  $58.3\text{ }^{\circ}\text{C}$ , relative deformation 18%). It was established that the polymer system pectin-chitosan has a higher sorption capacity for  $\text{Cu}^{2+}$  and  $\text{Ag}^{+}$  cations compared to other complexes. In particular, for  $\text{Cu}^{2+}$   $A=2.45\text{ mmol/g}$ , for  $\text{Ag}^{+}$   $A=3.8\text{ mmol/g}$ .

The obtained results confirm the promising use of polyelectrolyte complexes based on polysaccharides as effective materials for creating environmentally friendly membranes for wastewater filtration.

---

**KEYWORDS:** Polyelectrolyte complexes, Membranes, Water purification

---

**ACKNOWLEDGEMENTS:** The work was carried out with the financial support of a grant from the National Research Foundation of Ukraine "Formation and research of biopolymer membranes based on polyelectrolyte complexes and silver nanoparticles, promising for nanofiltration" (Application ID 2025.02/0018).

## Influence of detonation spraying parameters on the structure and properties of Al<sub>2</sub>O<sub>3</sub> coatings

A. Nabioldina<sup>1</sup>\*, D. Buitkenov<sup>1</sup>, Z. Sagdoldina<sup>1</sup>

1) Sarsen Amanzholov East Kazakhstan University, Ust-Kamenogorsk, Kazakhstan, Kazakhstan

\* anabioldina AT vku.edu.kz

The present study investigates the influence of detonation spraying parameters on the structure and properties of Al<sub>2</sub>O<sub>3</sub> coatings deposited on 10Kh18N9 stainless steel. The coatings were produced using a CCDS<sub>2000</sub> detonation system at different barrel filling ratios (53%, 58%, and 63%), allowing variation of the process energy parameters. A comprehensive analysis of the phase composition, microstructure, mechanical, tribological, and corrosion properties of the coatings was carried out. It was established that  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> is the dominant phase in all samples, with a content of 77-80%, which is attributed to the high temperatures of the detonation process. The coatings exhibit a dense and homogeneous structure with a well-defined interface with the substrate. The optimal mechanical properties were achieved at a barrel filling ratio of 58%, where the Young's modulus reached 190 GPa and the hardness was 1362 HV, due to the formation of the most compact structure. This regime also provided the highest adhesion strength. It was shown that the coatings significantly improve the corrosion resistance of the steel by reducing the corrosion current density and corrosion rate. Tribological tests revealed that wear resistance strongly depends on the counterbody material: minimal wear was observed when using ZrO<sub>2</sub>, whereas the use of 100Cr6 steel resulted in increased wear intensity. The obtained results demonstrate that optimization of detonation spraying parameters can significantly enhance the performance characteristics of Al<sub>2</sub>O<sub>3</sub> coatings, making them promising for the protection of structural materials.

**KEYWORDS:** Detonation spraying, Al<sub>2</sub>O<sub>3</sub> coating, Aluminum oxide, Phase composition, 10Kh18N9 steel

**ACKNOWLEDGEMENTS:** This research has been funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No.BR24992876)

### REFERENCES

- [1] V. P. Singh, A. Sil, and R. Jayaganthan, “Wear of Plasma Sprayed Conventional and Nanostructured Al<sub>2</sub>O<sub>3</sub> and Cr<sub>2</sub>O<sub>3</sub>, Based Coatings,” *Trans Indian Inst Met*, vol. 65, no. 1, pp. 1-12, Feb. 2012, doi: 10.1007/s12666-011-0070-0.
- [2] B. Rakhadilov, D. Kakimzhanov, D. Baizhan, G. Muslimanova, S. Pazylbek, and L. Zhurerova, “Comparative Study of Structures and Properties of Detonation Coatings with  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> and  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> Main Phases,” *Coatings*, vol. 11, no. 12, p. 1566, Dec. 2021, doi: 10.3390/coatings11121566.
- [3] V. V. Sirota, S. V. Zaitsev, M. V. Limarenko, D. S. Prokhorenkov, and A. S. Churikov, “Effect of powder morphology on the structure and properties of Al<sub>2</sub>O<sub>3</sub> based coatings obtained by detonation spraying,” *Construction materials and products*, vol. 7, no. 5, pp. 7-7, Oct. 2024, doi: 10.58224/2618-7183-2024-7-5-7.
- [4] D. Buitkenov, Z. Sagdoldina, A. Nabioldina, and C. Drenda, “The Study of Tribological Characteristics of YSZ/NiCrAlY Coatings and Their Resistance to CMAS at High Temperatures,” *Applied Sciences*, vol. 15, no. 14, p. 8109, Jan. 2025, doi: 10.3390/app15148109.

## Packaging polymer materials with antimicrobial activity

V. Demchenko<sup>1\*</sup>, A. Marynin<sup>2</sup>, M. Iurzhenko<sup>1</sup>, D. Shtepa<sup>2</sup>

1) E.O. Paton Electric Welding Institute of the National Academy of Sciences of Ukraine, Ukraine

2) National University of Food Technology, Ukraine

\* dvaleriy AT ukr.net

The creation and research of packaging materials based on biopolymers with silver nanoparticles is an urgent task today.

The relevance of packaging materials is due to their important role in maintaining the quality and safety of products, protecting them from external factors and extending the shelf life. The growth of e-commerce and logistics increases the demand for effective packaging, while environmental problems stimulate the development of biodegradable and recyclable materials. Thus, this area is of significant scientific and practical importance.

Using the wide-angle radiography method, it was established that the studied film materials have a semi-crystalline structure and the presence of Ag particles in the formed polymer matrices was confirmed. Morphological analysis of the studied samples showed that a layer of silver nanoparticles with a thickness of ~ 100 nm is formed on the surface of the biopolymer film made of polylactide (spraying time 5 min) with an average size of 5.9 nm; a layer of Ag particles with a thickness of ~ 425 nm is formed on the surface of polymer films based on polylactide and polycaprolactone (PLA-PCL) (spraying time 5 min). It was found that spraying silver nanoparticles on the surface of film packaging biopolymers PLA-PCL leads to a decrease in their temperature of onset of thermal destruction by 6.5 °C. According to differential scanning calorimetry, it was found that as a result of sputtering silver nanoparticles onto the surface of PLA-PCL polymers, the degree of crystallinity increases from 35% to 39%, as well as the melting temperature  $T_m$  from 168 °C to 169-170 °C. This effect is associated with the effect of silver particles that penetrate the polymer film to a certain depth and create a nucleating effect during polymer crystallization. In this case, there is no effect of a thin layer of silver nanoparticles on the amorphous phase of the polymer film, since the glass transition temperature of the polymer matrix ( $T_g$ ) does not change. It was found that biopolymer packaging materials based on polylactide and Ag nanoparticles (sputtering time 3 and 5 min) exhibited a bactericidal effect on microorganisms *S. aureus* and *E. coli* and were inactive against strains of *B. subtilis* and *P. aeruginosa*.

---

**KEYWORDS:** Polylactide, Polycaprolactone, Packaging films, Food products

---

**ACKNOWLEDGEMENTS:** The work was carried out with the financial support of a grant from the National Research Foundation of Ukraine "Development of packaging materials based on biopolymers with antimicrobial components of natural origin for long-term storage of food products" (Application ID 2025.07/0333).

## Antimicrobial PLA/PCL nanocomposite films incorporating silver nanoparticles for bread preservation

V. Demchenko<sup>1\*</sup>, A. Marynin<sup>2</sup>, N. Rybalchenko<sup>3</sup>, O. Stabnikova<sup>2</sup>

1) E.O. Paton Electric Welding Institute of the National Academy of Sciences of Ukraine, Ukraine

2) National University of Food Technology, Ukraine

3) D.K. Zabolotny Institute of Microbiology and Virology of the National Academy of Sciences of Ukraine, Ukraine

\* dvaleriy1 AT ukr.net

Bread, a staple food for much of the world's population, is highly perishable and prone to mold growth, limiting its shelf life and contributing to food waste. Furthermore, some molds, particularly those of the species *Aspergillus niger*, produce mycotoxins that are extremely harmful to human health. The use of packaging makes it possible to regulate bread storage conditions and to inhibit the rapid development of contaminating microflora. At the same time, packaging materials must meet a number of requirements, including cost-effectiveness, environmental sustainability, and effective antimicrobial performance. Recent advances in active packaging have focused on biodegradable materials with enhanced antimicrobial functionality achieved through the incorporation of antimicrobial agents such as silver nanoparticles, which inhibit microbial growth via their high surface area and multiple mechanisms of action, including membrane disruption and intracellular interactions [1].

The developed biodegradable PLA-PCL (80:20, w/w) packaging material incorporating silver nanoparticles (5.9 nm particle size, 97 m<sup>2</sup>/g specific surface area) via a spraying technique formed a ~100 nm-thick layer and demonstrated the potential to extend the shelf life of bakery products without compromising their quality. An additional enhancement of the antimicrobial properties of the resulting packaging material could be the addition of essential oil to its formula [2, 3]. The use of the developed packaging film reduced moisture loss and preserved crumb elasticity and hydration capacity in wheat bread during storage, consequently slowing the staling process. The use of the proposed packaging made it possible to extend the shelf life of bread by 2 days, while the packaged bread samples retained better freshness by 10% and 14% compared to the control samples after 24 and 48 hours of storage. PLA-PCL films with surface-deposited AgNPs demonstrated strong antimicrobial activity against *Staphylococcus aureus* and *Escherichia coli* (13.8-16.5 mm inhibition zones), while control films were inactive. In addition, the films effectively inhibited mold growth on bread samples inoculated with *Aspergillus niger* and *Penicillium chrysogenum* conidia.

Overall, the developed PLA-PCL biodegradable nanocomposite film incorporating silver nanoparticles demonstrated effective antimicrobial performance and the ability to extend the shelf life of bakery products without compromising their quality, highlighting its potential for application in active food packaging systems.

---

**KEYWORDS:** PLA-PCL films, AgNPs, Active packaging, Antimicrobial activity, Bread preservation

---

**ACKNOWLEDGEMENTS:** The work was carried out with the financial support of a grant from the National Research Foundation of Ukraine "Development of packaging materials based on biopolymers with antimicrobial components of natural origin for long-term storage of food products" (Application ID 2025.07/0333).

---

### REFERENCES

- [1] E.L.L. Garcia, O.A.A. Attallah, M. Mojicevic, D.M.M. Devine, and F.M. Brennan, "Antimicrobial active bioplastics using triangular silver nanoplate integrated polycaprolactone and polylactic acid films", *Materials.*, 4, 11322021 (2021).
- [2] N. Rybalchenko., V. Demchenko, T. Hnatiuk, O. Vasyliuk, M. Iurzenko, T. Rybalchenko, I. Sytnyk, D. Shtepa, and A. Marynin, "Antimicrobial effect of biopolymer packaging materials with silver nanoparticles for food storage", *Mikrobiol. Zh.*, 86, 30-41 (2024).
- [3] V. Demchenko, Y. Mamunya, I. Sytnyk, M. Iurzenko, I. Krivtsun, N. Rybalchenko, K. Naumenko, L. Artiukh, M. Kowalczyk, O. Demchenko, and A. Marynin, "Fabrication of polylactide composites with silver nanoparticles by sputtering deposition and their antimicrobial and antiviral applications", *Polym. Int.*, 74, 207-216 (2025).

## Effect of preliminary mechanical surface treatment on the kinetics of plasma-electrolytic nitriding of chromium-alloyed structural steel

A. Maulit<sup>1\*</sup>, Z. Satbayeva<sup>2</sup>, B. Rakhadilov<sup>3</sup>, A. Rustemov<sup>3</sup>

1) Shakarim State University of Semey, Kazakhstan

2) Shakarim University, Kazakhstan

3) PlasmaScience, Kazakhstan

\* maulit.almas AT gmail.com

Plasma-electrolytic nitriding (PEN) is a promising method for surface hardening of structural steels, enabling the formation of wear- and corrosion-resistant diffusion layers, while the kinetics of their formation is governed by both discharge parameters and the initial surface condition of the material [1,2]. It is well known that preliminary mechanical treatment (grinding, polishing, abrasive blasting) alters surface roughness, defect density, and residual stress levels in the surface layer, thereby significantly affecting mass transfer processes; for chromium-containing steels, oxide and carbonitride phases capable of forming diffusion barriers are of additional importance [3,4]. However, the influence of different types of mechanical surface preparation on the kinetics of PEN remains insufficiently studied. In this work, the effect of preliminary mechanical surface treatment on the growth kinetics of the nitrided layer during plasma-electrolytic nitriding of chromium-alloyed structural steel is investigated. Here, we show that an increase in surface roughness and defect density leads to an acceleration of the initial stage of nitriding and an increase in the thickness of the diffusion layer. It is established that samples subjected to mechanical treatment exhibit a higher layer growth rate following a parabolic law, due to an increased effective surface area and a higher number of diffusion paths, whereas polished surfaces are characterized by slower kinetics as a result of a reduced density of active sites and the formation of a stable oxide film. The obtained results refine the current understanding of the role of surface condition in plasma-electrolytic treatment processes and demonstrate the possibility of controlling diffusion processes through mechanical surface preparation. Thus, controlling the surface morphology and structural state is a key factor in optimizing PEN regimes and the properties of the formed layers. The results open up prospects for targeted control of nitrogen saturation kinetics by combining mechanical and plasma-electrolytic treatments, which can be used in the development of hardening technologies for machine components operating under severe wear and high-load conditions, as well as in the design of functional gradient layers with tailored performance characteristics.

**KEYWORDS:** Plasma-electrolytic nitriding, Preliminary mechanical treatment, Surface roughness, Diffusion kinetics, Chromium-alloyed structural steel

**ACKNOWLEDGEMENTS:** This research has been funded by the Committee of Science of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. BR24992870)

### REFERENCES

- [1] L. Shen, L. Wang, J.J. Xu, Y.C. Shan, Effect of pre-shot peening on plasma nitriding kinetics of austenitic stainless steel. *Advanced Materials Research*, 634, 2955-2959 (2013).
- [2] B. Rakhadilov, Z. Satbayeva, A. Maulit, R. Kozhanova, R. Kurmangaliyev, A. Rustemov, Comprehensive Study of Electrolytic Plasma Nitriding of Austenitic Stainless Steels. *Crystals* 2025, 15, 456. <https://doi.org/10.3390/cryst15050456>
- [3] Y. Lu, D. Li, H. Ma, X. Liu, M. Wu, J. Hu, Enhanced plasma nitriding efficiency and properties by severe plastic deformation pretreatment for 316L austenitic stainless steel. *Journal of Materials Research and Technology*, 15, 1742-1746 (2021).
- [4] N. Yamauchi, N. Ueda, K. Demizu, A. Okamoto, T. Sone, K. Oku, .. & Akamatsu, K. (2020). Effect of Peening as Mechanical Pre-Treatment on the Formation of S Phase in Plasma Nitrided 304 Austenitic Stainless Steel. In *Stainless Steel 2000* (pp. 247-261). CRC Press.

## Effect of reactive magnetron sputtering parameters on the structure and properties of $\text{TiO}_x\text{N}_y$ thin films

A. Kenesbekov<sup>1\*</sup>, A. Ashatov<sup>1</sup>, E. Turabekov<sup>1</sup>

1) D. Serikbayev East Kazakhstan Technical University, Kazakhstan

\* kenesbekovaidar AT gmail.com

Titanium oxynitride ( $\text{TiO}_x\text{N}_y$ ) coatings were deposited on 316L stainless steel substrates by reactive magnetron sputtering in an Ar- $\text{N}_2$ - $\text{O}_2$  gas mixture at a fixed N:O ratio of 1.6. The argon flow rate was considered as the key process parameter, and three sample series were prepared: Ar<sub>33</sub>, Ar<sub>25</sub>-28, and Ar<sub>26</sub> (sccm). The obtained coatings exhibited a dense and uniform microstructure, with thicknesses ranging from 2.13 to 5.51  $\mu\text{m}$  depending on the deposition conditions. X-ray diffraction analysis revealed a multiphase structure consisting of TiN,  $\text{TiO}_x\text{N}_y$ , and TiO phases, which is typical for titanium oxynitride coatings. Mechanical and tribological tests demonstrated a strong dependence of properties on deposition parameters. The lowest friction coefficient ( $\mu \approx 0.26$ - $0.28$ ) was observed for the Ar<sub>26</sub> series, indicating optimal deposition conditions. Electrochemical measurements in 3.5 wt.% NaCl solution showed that the highest corrosion resistance was achieved for the Ar<sub>25</sub>-28 series ( $i_{\text{corr}} = 2.82 \times 10^{-7}$  A/cm<sup>2</sup>;  $v_{\text{corr}} = 0.00573$  mm/year).

All coatings exhibited a hydrophilic surface with a contact angle of  $\sim 50$ - $57^\circ$ , which is beneficial for biomedical applications. The results demonstrate that controlling the argon flow rate during reactive magnetron sputtering enables targeted tuning of the structure and functional properties of  $\text{TiO}_x\text{N}_y$  coatings, making them promising for surface modification of vascular implants [1].

---

**KEYWORDS:** Titanium oxynitride, Thin protective coatings, Biocompatible surfaces, Corrosion resistance, Mechanical properties

---

**ACKNOWLEDGEMENTS:** This research was funded by the Committee of Science of the Ministry of Science and Higher Education of the Republic of Kazakhstan. (Grant No. BR24992862).

---

### REFERENCES

- [1] A. Kengesbekov, B. Rakhadilov, A. Kussainov, A. Serikbaikyzy, A. Askhatov, Z. Aringozhina, Formation of Titanium Oxynitride Films by Reactive Magnetron Sputtering, Their Structural Features and Properties. *Coatings*, 15(12), 1434 (2025).

## Effect of soluble and insoluble silicates on the formation and structure of phosphate-based PEO coatings on magnesium

Y. Husak<sup>1\*</sup>, V. Grebnevs<sup>2</sup>, V. Deineka<sup>3</sup>, P. Shubin<sup>4</sup>, A. Maciej<sup>2</sup>, W. Simka<sup>5</sup>

1) Biomedical Research Center, Academic and Research Medical Institute, Sumy State University, Sumy, Ukraine

2) Silesian University of Technology, Faculty of Chemistry, Poland

3) Institute of Atomic Physics and Spectroscopy, University of Latvia, Latvia

4) University of Latvia, Riga, Latvia

5) Silesian University of Technology, Faculty of Chemistry, Gliwice, Poland

\* evgenia.husak AT gmail.com

Magnesium and its alloys are promising materials for biodegradable implants due to their favorable mechanical properties and biocompatibility [1]. However, their rapid corrosion rate significantly limits their clinical application. Plasma electrolytic oxidation (PEO) is a surface modification technique that can enhance corrosion resistance while maintaining biocompatibility [2]. In particular, mixed phosphate-silicate electrolytes involve complex plasma-chemical and electrochemical interactions that strongly influence coating formation kinetics, microstructure, and biological performance. Although silicate-based systems have been widely studied, including both soluble (SS) and insoluble silicates (IS), their comparative effects in combination with different phosphate species remain insufficiently understood [3, 4].

Therefore, the aim of this work is to investigate the properties of coatings formed in electrolytes containing soluble and insoluble silicates, in combination with phosphates.

For PEO treatment of Mg-based implants, we developed three electrolyte formulations: we elaborated following electrolyte composition: SS<sub>1</sub> containing 5 g·dm<sup>-3</sup> Na<sub>2</sub>SiO<sub>3</sub> and 15 g·dm<sup>-3</sup> Na<sub>3</sub>PO<sub>4</sub>, SS<sub>2</sub> - 5 g·dm<sup>-3</sup> Na<sub>3</sub>PO<sub>4</sub> and 3 g·dm<sup>-3</sup> KOH, and IS<sub>1</sub> - 5 g·dm<sup>-3</sup> Na<sub>3</sub>PO<sub>4</sub>, 3 g·dm<sup>-3</sup> KOH, and 50 g·dm<sup>-3</sup> CaSiO<sub>3</sub>. The PEO process was conducted under an impulse current up to with a fixed voltage (in 250V, 300V, and 350V), employing with the use of a high-voltage power supply (PWR 800H, Kikusui, Japan). The obtained resulting samples were analyzed by scanning electron microscopy equipped with energy-dispersive X-ray spectroscopy (EDX). The surface wettability was measured by static contact angle (CA) measurements. Cytocompatibility of the PEO coatings was evaluated using MG-63 cells, and cell viability was assessed after 1, 3, and 6 days using a resazurin reduction assay relative to uncoated control samples.

The results demonstrated that soluble silicates significantly accelerated coating formation, while systems containing insoluble silicate particles required higher voltages (up to 350 V). The obtained coatings exhibited a porous morphology. Increased P content led to thicker coatings for the SS<sub>1</sub> sample (3.8 ± 0.7 μm) at 250 V. EDX analysis demonstrated effective incorporation of P, reaching up to 7 at.% for SS<sub>1</sub> at 250 V and for SS<sub>2</sub> and SS<sub>3</sub> at 350 V. Higher Si content was observed only for soluble silicate systems. However, the synergistic effect of insoluble silicates and phosphates improved surface hydrophilicity at higher applied voltages for the SS<sub>3</sub> sample (CA down to ~20°). Biological studies using MG-63 cells indicated that selected coatings, particularly SS<sub>1</sub> and SS<sub>2</sub> formed at higher voltages in particle-containing electrolytes, exhibited cytocompatible properties.

The study highlights the distinct roles of soluble and insoluble silicates in tailoring coating properties.

---

**KEYWORDS:** Magnesium, Biodegradable implants, PEO coating, Phosphate, Silicate

---

**ACKNOWLEDGEMENTS:** Latvian Council of Science Project (Grant lzp-2024/1-0135)

### REFERENCES

- [1] Y. Zhang, S. Zhang, H. Li, C. Liu, H. Wang, and L. Ma, "Magnesium Silicate Coatings Were Prepared by Micro-Arc Oxidation on the Surface of Magnesium Alloys Through the Synergistic Effect of SiO<sub>3</sub><sup>2-</sup>/F<sup>-</sup>", *Materials (Basel)*, vol 18, no 20, (2025).
- [2] J. Wang *et al.*, "Corrosion resistance and biodegradability of micro-arc oxidation coatings with the variable sodium fluoride concentration on ZM21 magnesium alloys", *J. Alloys Compd.*, vol 962, (2023).
- [3] J. Liang, P. B. Srinivasan, C. Blawert, M. Störmer, and W. Dietzel, "Electrochemical corrosion behaviour of plasma electrolytic oxidation coatings on AM50 magnesium alloy formed in silicate and phosphate based electrolytes", *Electrochim. Acta*, vol 54, no 14, pp 3842-3850, (2009).
- [4] Y. M. Wang *et al.*, "A metasilicate-based ceramic coating formed on magnesium alloy by microarc oxidation and its corrosion in simulated body fluid", *Surf. Coatings Technol.*, vol 219, pp 8-14, (2013)..

## An experimental and theoretical investigation of size effects in electrical resistivity of FeNi(Co) thin-film alloys

O. Pylypenko<sup>1</sup>, D. Saltykov<sup>2</sup>, I. Volk<sup>1</sup>, I. Pazukha<sup>1\*</sup>, Y. Shkurdoda<sup>1</sup>

1) Sumy State University, Ukraine

2) Sumy State Pedagogical University Named After A.S. Makarenko, Romens'ka St. 87, 40002 Sumy, Ukraine

\* i.pazuha AT aph.sumdu.edu.ua

Among various magnetic alloys, Fe-based thin-film alloys, particularly the binary alloys  $\text{Fe}_x\text{Ni}_{1-x}$  and  $\text{Fe}_x\text{Co}_{1-x}$ , have received considerable attention. To date, a significant amount of experimental and theoretical work has been accumulated on the study of the structural and phase state, electrical conductivity, magnetic, and magnetoresistive properties of  $\text{Fe}_x\text{Ni}_{1-x}$  and  $\text{Fe}_x\text{Co}_{1-x}$  [1-3]. Besides, the electrical properties of thin-film alloys are as important as the magnetic ones. The resistivity value significantly depends on the method and technological conditions used to obtain film alloys.

Binary thin-film alloys  $\text{Fe}_x\text{Ni}_{1-x}$  and  $\text{Fe}_x\text{Co}_{1-x}$  with nominal thickness ( $d$ ) ranging from 15 to 80 nm were deposited using electron-beam evaporation in a high vacuum chamber maintained at a base pressure of  $10^{-4}$  Pa. Bulk alloys  $\text{Fe}_x\text{Ni}_{1-x}$  and  $\text{Fe}_x\text{Co}_{1-x}$  with compositions  $x = 0.2-0.8$  served as source materials. Condensation was performed at room temperature (RT) with deposition rates of 0.5-1 nm/s. Film thickness was monitored "in-situ" using a quartz resonator with an accuracy of  $\pm 5\%$ . Following deposition, all samples underwent annealing at  $T_{\text{ann}} = 700$  K.

Structural characterization revealed that both alloy systems undergo composition-dependent phase transitions upon annealing at 700 K. For  $\text{Fe}_x\text{Ni}_{1-x}$  thin-film alloys, the transition from fcc to bcc structure occurs at  $x \approx 0.6$ , while  $\text{Fe}_x\text{Co}_{1-x}$  films transform from mixed bcc+fcc to single bcc phase at  $x \approx 0.3$ . The mean grain size exhibits a linear relationship with film thickness ( $L \approx k \times d$ ), with proportionality constants ranging from 0.6 to 2.0 for  $\text{Fe}_x\text{Ni}_{1-x}$  and 0.75 to 1.5  $\text{Fe}_x\text{Co}_{1-x}$ , depending on composition. Electrical transport measurements demonstrated classical metallic thin-film behavior across the investigated thickness range (15-80 nm). Both alloy systems show a monotonic decrease in resistivity and a corresponding increase in temperature coefficient of resistance with increasing film thickness, approaching asymptotic values characteristic of bulk materials. Theoretical analysis using the Tosser-Tellier models conclusively identified grain boundary scattering as the dominant mechanism controlling electrical conductivity in these polycrystalline films. The surface scattering parameter  $p$  remains below 0.036 for all investigated compositions, indicating nearly complete diffuse scattering at external surfaces with minimal contribution to overall resistivity. In contrast, reflection coefficients at grain boundaries range from 0.15 to 0.40, indicating a strong dependence on crystallite size and a direct correlation with observed resistivity variations. These studies demonstrate that electrical transport properties can be effectively controlled by manipulating grain size and thin-film thickness, providing valuable insights for designing spintronic devices based on nanostructured magnetic thin films.

**KEYWORDS:** Thin-film alloys, Electrical resistivity, Size effects, Grain boundary scattering, Temperature coefficient of resistance

**ACKNOWLEDGEMENTS:** Funded by the NATO Program "Science for Peace and Security" (project number G6131) and the State Program of the Ministry of Education and Science of Ukraine (project numbers: 0224U033036, 0126U000589).

### REFERENCES

- [1] Shih-Hung Lin, Yung-Huang Chang, Wei-Chiao Chen, Huang-Wei Chang, "Influence of annealing temperature and polymer substrate type on the structural, magnetic, mechanical, and electrical properties of  $\text{Ni}_{80}\text{Ce}_{20}$  thin films for flexible electronics applications", *J. Alloys Compd.*, 1038, 182623 (2025).
- [2] M. Zhang, C. Deng, "Magnetic, optical and electrical properties of permalloy films by DC magnetron sputtering", *J. Mater. Sci.: Mater. Electron.*, 32, 4949 (2021).
- [3] J. Marciniak, M. Werwiński, "Magnetic anisotropy of L10 FeNi (001), (010), and (111) ultrathin films: A first-principles study", *J. Magn. Magn. Mater.*, 609, 172455 (2024).

## The effect of laser surface hardening on the microstructural characteristics and wear resistance of 9CrSi steel

S. Bolatov<sup>1</sup>\*

1) Sarsen Amanzholov East Kazakhstan University, Ust-Kamenogorsk, Kazakhstan, Kazakhstan

\* sanzharbolatov94 AT gmail.com

Laser surface hardening is a widely used technique for enhancing the wear resistance and durability of tool steels without affecting their bulk properties. It enables localised heat treatment with high precision and minimal thermal distortion. However, the relationship between processing parameters and the resulting microstructure and performance is not well understood for high-carbon chromium steels such as 9CrSi.

In particular, the combined influence of laser power, modulation frequency and scanning speed on microstructure-property-performance relationships has not yet been fully clarified.

In this study, we demonstrate that laser surface hardening of 9CrSi steel produces a martensitic surface layer containing varying amounts of retained austenite, which significantly improves the material's mechanical and tribological properties.

We found that laser processing increases surface microhardness from ~220 HV<sub>0.1</sub> to 950-1000 HV<sub>0.1</sub> and reduces the wear rate by more than an order of magnitude under dry sliding conditions. Depending on the processing regime, the hardened layer thickness varies from ~500 to 750 μm, and X-ray diffraction confirms the formation of α'-Fe, γ-Fe, and Fe<sub>3</sub>C phases with increased lattice microstrain.

These results demonstrate that scanning speed plays a key role in controlling thermal input, microstructure refinement and hardened layer depth, while the balance between martensite and retained austenite governs friction and wear behaviour. Overall, this study establishes a parameter-microstructure-performance map for laser-hardened 9CrSi steel, providing guidance on how to optimise processing regimes to improve wear resistance and mechanical performance in engineering applications.

---

**KEYWORDS:** Laser surface hardening, 9CrSi steel, Microstructure evolution, Retained austenite, Dry sliding friction

---

**ACKNOWLEDGEMENTS:** This research was funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. BR24992876).

---

### REFERENCES

- [1] Z. Sagdoldina, L. Zhurerova, Y. Tyurin, D. Baizhan, A. Kuykabayeva, S. Abildinova, R. Kozhanova, Modification of the Surface of 40 Kh Steel by Electrolytic Plasma Hardening. *Metals* 2022, 12, 2071.
- [2] L. Záhon, Kuchar, J.; J. Horník; Krc'íl, J.; Kudláček, J. Laser Surface Hardening of Austempered Ductile Iron (ADI). *Coatings* 2024, 14, 958.
- [3] L. Bayatanova, B. Rakhadilov, S. Kurbanbekov, M. Skakov, N. Popova, Fine Structure of Low-Carbon Steel after Electrolytic Plasma Treatment. *Mater. Test.* 2021, 63, 842-847.
- [4] N. Li, S. Elattar, L. Xu, M. Hussien, Y. Alqurashi, T. Saidani, Effective Prediction of Temperature Gradient and Thermal Softening Characterizations in Heat Affected Zone in Low Frequency Pulsed Laser Assisted Turning Process of Hardened Steel Parts. *Opt. Laser Technol.* 2026, 194, 114400.
- [5] B. Rakhadilov, Z. Satbayeva, D. Baizhan, Effect of electrolytic-plasma surface strengthening on the structure and properties of steel 40kHN. In *Proceedings of the METAL 2019-28th International Conference on Metallurgy and Materials*, Brno, Czech Republic, 22-24 May 2019; pp. 950-955.
- [6] B.K. Rahadilov, L.G. Zhurerova, Z.B. Sagdoldina, A.B. Kenesbekov, L.B. Bayatanova, Morphological Changes in the Dislocation Structure of Structural Steel 20GL after Electrolytic-Plasma Hardening of the Surface. *J. Surf. Investig. X-Ray Synchrotron Neutron Tech.* 2021, 15, 408-413.
- [7] D. Baizhan, B. Rakhadilov, L. Zhurerova, Y. Tyurin, Z. Sagdoldina, M. Adilkanova, R. Kozhanova, Investigation of Changes in the Structural-Phase State and the Efficiency of Hardening of 30CrMnSiA Steel by the Method of Electrolytic Plasma Thermocyclic Surface Treatment. *Coatings* 2022, 12, 1696.
- [8] C. He, X. Hu, S. Qu, Z. Chen, Z. Tang, H. Xiao, B. Lin, F. Lai, Synergistic Strengthening Effect of Discrete Laser Surface Hardening and Ultrasonic Surface Rolling on the Wear and Fatigue Behaviors of Cr-Ni-Mo Steel. *Surf. Coat. Technol.* 2025, 517, 132873.
- [9] H. Sun, Y. Han, M. Du, B. Song, Z. Sun, R. Lang, Effect of Strain Hardening and Martensite Phase Transformation on Residual Stress in 30MnCrNiMo High-Strength Steel Laser-MAG Hybrid Welding. *Mater. Today Commun.* 2025, 48, 113473.
- [10] Z. Satbayeva, A. Maulit, N. Ispulov, D. Baizhan, B. Rakhadilov, R. Kusainov, Electrolytic Plasma Nitriding of Medium-Carbon Steel 45 for Performance Enhancement. *Crystals* 2024, 14, 895.

## Oxygen-tolerant SI-ARGET ATRP synthesis of antifouling zwitterionic terpolymer brush nanocoatings

A. Pilipenco-Šleichertová<sup>1</sup>\*, V. Cirik<sup>1</sup>, O. Romanyuk<sup>2</sup>, L. Fekete<sup>1</sup>, M. Valášková<sup>3</sup>, N. S. L. Jr<sup>1</sup>,  
H. Vaisocherová-Lísalová<sup>1</sup>

1) FZU - Institute of Physics of the Czech Academy of Sciences, Na Slovance 2, 180 00 Prague, Czech Republic, Czech Republic

2) FZÚ - Institute of Physics, Czech Academy of Sciences, Cukrovarnická 10, 162 00 Prague 6, Czech Republic

3) FZU - Institute of Physics of the Czech Academy of Sciences, Na Slovance 2, 180 00 Prague, Czech Republic, Czech Republic

\* sleichertova AT fzu.cz

Biofouling is a major limitation for nanomaterials exposed to complex biological, environmental, and technological media. Nonspecific adsorption of proteins, cells, microorganisms, and matrix components can substantially change surface properties, block designed interfacial functions, and reduce the lifetime and reliability of devices.

Polymer brush nanocoatings are promising antifouling materials because their dense and highly hydrated architecture can minimize nonspecific interactions while preserving chemical functionality. Random terpolymer brushes composed of *N*-(2-hydroxypropyl) methacrylamide (HPMAA), carboxybetaine methacrylamide (CBMAA), and sulfobetaine methacrylamide (SBMAA) have shown excellent resistance to fouling and compatibility with biofunctionalization [1, 2]. However, their synthesis typically relies on surface-initiated atom transfer radical polymerization (SI-ATRP) under inert conditions, which complicates experimental handling and may limit reproducibility and scalability.

Here, we report the first synthesis of poly(HPMAA-*co*-CBMAA-*co*-SBMAA) terpolymer brushes via surface-initiated activators regenerated by electron transfer atom transfer radical polymerization (SI-ARGET ATRP) and compare this approach with classical SI-ATRP. The ARGET method enables polymerization under significantly relaxed conditions, without strict oxygen exclusion, simplifying experimental handling and improving robustness.

The coatings were characterized by infrared spectroscopy (IR), X-ray photoelectron spectroscopy (XPS), water contact angle measurements, atomic force microscopy (AFM), and spectroscopic ellipsometry to assess their chemical composition, wettability, morphology, and thickness. Their resistance to nonspecific fouling was evaluated using human blood plasma as a complex biological challenge, and preservation of functional interfacial performance after biofunctionalization was examined using *Vibrio cholerae* O<sub>1</sub> Ogawa as a bacterial model. This comparison evaluates whether a less oxygen-sensitive polymerization route can produce zwitterionic terpolymer brush nanocoatings with physicochemical properties and antifouling performance comparable to coatings prepared by conventional SI-ATRP.

By linking polymerization strategy, nanoscale coating structure, chemical composition, and resistance to complex media fouling, this work supports SI-ARGET ATRP as a practical route for scalable fabrication of antifouling nanomaterials.

---

**KEYWORDS:** Polymer brush, Antifouling surfaces, Zwitterionic nanomaterials, SI-ARGET ATRP, Surface functionalization

---

**ACKNOWLEDGEMENTS:** The results presented in this work are part of the project Biosensor Technology for Citizen Safety: An Adaptable Solution for Field Deployment (VB02000070), supported by the Ministry of the Interior of the Czech Republic through the program Open Calls for Security Research of the Czech Republic 2021-2026: Development, Testing and Evaluation of New Security Technologies (SECTECH). This work was further supported by the Czech Science Foundation under grant numbers 24-10671S and 22-20012S, and by the Programme Johannes Amos Comenius of the Ministry of Education, Youth and Sports of the Czech Republic, project SENDISO (No. CZ.02.01.01/00/22\_008/0004596).

---

### REFERENCES

- [1] A. Pilipenco, G. Subbiahdoss *et al.*, “Fine-tuned functionalizable terpolymer brush nanocoating resists protein adsorption and bacterial adhesion while promoting macrophage activity and osteoblast proliferation.” *ACS Applied Materials & Interfaces* 17, 65399-65410 (2025).
- [2] M. Forinová, A. Pilipenco *et al.*, “Functionalized terpolymer-brush-based biointerface with improved antifouling properties for ultra-sensitive direct detection of virus in crude clinical samples.” *ACS Applied Materials & Interfaces* 13, 60612-60624 (2021).

## Refractory multicomponent protective thin films for bioactive environments

B. Postolnyi<sup>1, 2 \*</sup>, A. Sobetkii<sup>3</sup>, A. Talipova<sup>4</sup>, R. Basnukaeva<sup>5</sup>, A. Pogrebnjak<sup>2, 6</sup>

1) Institute of Physics for Advanced Materials, Nanotechnology and Photonics, Faculty of Sciences, University of Porto, Portugal

2) Sumy State University, Ukraine

3) MGM Star Construct, Romania

4) Al-Farabi Kazakh National University, Kazakhstan

5) B. Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine, Ukraine

6) National Research-Development Institute for Non-Ferrous and Rare Metals - IMNR, Romania

\* b.postolnyi AT gmail.com

Refractory multicomponent thin films are of growing interest as protective surface materials for demanding environments where mechanical stability, corrosion resistance, and biological surface interactions may be simultaneously required. In this work, thin films based on WNbTa, WMoRe, and TiWV(Mo,Zr,Nb) systems were considered as potential multifunctional coatings for bioactive environments.

The films were produced by magnetron sputtering under vacuum conditions, using high-power deposition at a low deposition rate. Coatings with thicknesses of approximately 200-300 nm were deposited on different substrates, including Si single crystal, glass, and TiVAI titanium alloy, and analysed using complementary structural, compositional, morphological, mechanical, tribological, corrosion-related, and microbiological characterization methods. These included SEM/EDS, RBS/PIXE elemental depth profiling, AFM surface morphology analysis, XRD phase and microstructure analysis, nanohardness and elastic modulus measurements, ball-on-disk wear testing, corrosion assessment, and antimicrobial evaluation. Particular attention was given to the relationship between coating composition, surface state, and possible functional response under conditions relevant to protective and bioactive applications.

The study provides a comparative basis for assessing refractory-metal-based multicomponent thin films as candidates for advanced protective coatings. Among the investigated systems, the WNbTa film exhibited the highest hardness, reaching about 13 GPa, while the WMoRe film showed the lowest hardness but demonstrated the most promising antibacterial properties. This contrast suggests that mechanical durability and biological surface response may be composition-dependent and should be considered together when designing multifunctional refractory coatings. The obtained results are discussed in terms of their potential for surface durability and control of microbial interactions, supporting further development of such coatings for bioactive and corrosive environments.

---

**KEYWORDS:** Refractory multicomponent thin films, Magnetron sputtering, Protective coatings, Antimicrobial activity

## Laser-fabricated nanostructured titanium grids and their chemical modification for photocatalytic and SERS applications

J. Kisała<sup>1</sup>, A. Barylyak<sup>2</sup>, Y. Bobitski<sup>1\*</sup>

1) Faculty of Exact and Technical Sciences, University of Rzeszow, Pigońia 1 Str., 35-310 Rzeszow, Poland

2) Danylo Halytsky Lviv National Medical University, Pekarska Str. 69, 79010 Lviv, Ukraine

\* ybobytsky AT ur.edu.pl

Safeguarding environmental quality is a prerequisite for sustainable development, driving the need for efficient systems that remove organic pollutants from water and enable trace-level molecular detection. Therefore, systems for cleaning pollutants and methods for detecting and identifying trace molecular quantities of substances are of justified interest. In this regard, the potential of catalysis and Surface-enhanced Raman Scattering (SERS) is undeniable. We present laser-fabricated titanium grids that are subsequently modified by silver nanoparticle deposition and controlled surface oxidation to operate simultaneously as photocatalysts and SERS-active substrates. We demonstrate that oxidation of laser-perforated grids, which substantially enriches the surface with oxygen, yields the highest degradation rate of methylene blue, whereas grids modified with plasmonic silver nanostructures exhibit strong SERS activity due to their well-controlled nanoparticle architecture. Morphological and compositional analyses reveal that distinct modification protocols produce different silver nanoparticle arrangements and oxide layers, which directly govern photocatalytic efficiency and electromagnetic-field enhancement. The porous three-dimensional microarchitecture of the grids provides a large specific surface area and facilitates efficient analyte adsorption, further amplifying SERS sensitivity. By integrating scalable laser processing with simple wet-chemical treatments, this work establishes a versatile route to multifunctional titanium grids for water purification and molecular sensing and proposes design principles that can be extended to other pollutants and probe molecules.

---

**KEYWORDS:** Laser-fabricated titanium grids, Photocatalysis, Surface-enhanced Raman scattering, Silver nanoparticles

---

### REFERENCES

- [1] P. Krzemiński, A. Lazauskas, S. Meskinis, R. Wojnarowska-Nowak, B. Cieniek, Y. Bobitski, J. Kisała, "Nanosecond Laser-Fabricated Titanium Meshes and Their Chemical Modification for Photocatalytic and SERS Applications," *Appl. Sci. (Basel)* 15(21), 11579 (2025).

# Track 6

## Ultrawide Bandgap Materials and Nanophotonics

## Radiation-induced defects in wide-bandgap semiconductors: Formation, evolution, and impact on device performance

P. A. Jóźwik<sup>1\*</sup>, K. Lorenz<sup>2</sup>, E. Grzanka<sup>3</sup>, R. Ratajczak<sup>1</sup>, C. Mieszczyński<sup>1</sup>, J. Matulewicz<sup>1</sup>, M. Grabowski<sup>3</sup>, A. Caçador<sup>2</sup>, F. Garrido<sup>4</sup>, A. Turos<sup>1</sup>

1) National Centre for Nuclear Research, Otwock, Poland, Poland

2) INESC Microsystems and Nanotechnology, Lisboa, Portugal, Portugal

3) Institute of High Pressure Physics, Polish Academy of Sciences, Warsaw, Poland, Poland

4) Université Paris-Saclay, CNRS/IN2P3, IJCLab, Orsay, 91405, France, France

\* przemyslaw.jozwik AT ncj.gov.pl

Wide bandgap semiconductors (WBGs) are of pivotal importance to the development of next generation power electronics, sensors and high frequency devices. However, the performance and long-term reliability of the devices are significantly impacted by radiation-induced defects arising during ion implantation, device processing or operation in harsh environments. It is therefore essential to understand how these defects form, evolve, and degrade material properties if stable device functionality is to be ensured.

From a materials science perspective, ion bombardment introduces a hierarchy of structural defects, ranging from point defects to extended dislocation networks. The formation pathways of these defects depend sensitively on crystal structure, polarity, and composition. Thus, only the combination of different techniques such as Rutherford backscattering spectrometry in channeling mode (RBS/C), X-ray diffraction (XRD), and transmission electron microscopy (TEM) provide complementary insights into the processes of disorder accumulation and strain buildup.

The core issue addressed in this talk pertains to the process by which defects induced by radiation accumulate and transform in WBGs, thereby constraining device efficiency and operational lifetime. In this study, we demonstrate the efficacy of integrating RBS/C with McChasy modelling in enabling quantitative identification of defect types and their growth mechanisms in GaN, AlGaN, SiC, and Ga<sub>2</sub>O<sub>3</sub> subjected to controlled ion irradiation. However, analytical models frequently lack the capacity to differentiate between various defect types, thus necessitating the employment of advanced Monte Carlo simulations such as McChasy [1]. These simulations explicitly model displaced atoms, dislocation loops, and their fluence-dependent evolution.

The results obtained demonstrate that defect formation in GaN is polarity-dependent, with Ga-polar and N-polar orientations exhibiting distinct defect concentrations and annealing behaviour. The initial observation of dislocations and dislocation loops in AlGaN enabled the development of a dedicated dislocation model implemented in the McChasy code [2]. In SiC, self-implantation with Si and C ions is used as a surrogate for neutron irradiation, thereby enabling the controlled modelling of neutron-induced damage pathways [3]. In the monoclinic β-Ga<sub>2</sub>O<sub>3</sub>, ion bombardment has been shown to induce significant structural transformations, including strain-mediated defect clustering and symmetry-related lattice rearrangements [4].

These effects directly impact the design of radiation-tolerant power devices, high-frequency transistors, and sensors operating in space, nuclear, or high-temperature environments. This work demonstrates more generally how integrating experiments with physics-based simulations advances the ability to predict material degradation pathways. What, in turn, supports the development of robust nanomaterials and reliable electronic technologies.

---

**KEYWORDS:** Wide-bandgap semiconductors, Ion-beam-induced defects, Defect modeling, Radiation damage, Device reliability

---

**ACKNOWLEDGEMENTS:** The GaN work was co-financed by the Polish Ministry of Education and Science upon the bilateral project 5240/LATR/2022/0 between NCBJ, Poland, and LATR, Portugal. Transnational access to the LATR facility was also supported by the EU Research and Innovation program HORIZON 2020 (RADIATE) under Grant Agreement 23003122-ST and 23003121-ST as well as by the proposal 34616 of the ReMade@ARI project (<https://doi.org/10.3030/101058414>), funded by the European Union as part of the Horizon Europe call HORIZON-INFRA-2021-SERV-01 under grant agreement number 101058414 and co-funded by UK Research and Innovation (UKRI) under the UK government's Horizon Europe funding guarantee (grant number 10039728) and by the Swiss State Secretariat for Education, Research and Innovation (SERI) under contract number 22.00187. Views and opinions expressed are however those of the authors only and do not necessarily reflect those of the European Union or the UK Science and Technology Facilities Council or the Swiss State Secretariat for Education, Research and Innovation (SERI). Neither the European Union nor the granting authorities can be held responsible for them. The Ga<sub>2</sub>O<sub>3</sub> research was carried out within the project UMO-2022/45/B/ST5/02810 financed by National Science Centre, Poland.

---

### REFERENCES

- [1] P. Jóźwik, A. Caçador, K. Lorenz, R. Ratajczak, and C. Mieszczyński, "Monte Carlo simulations of ion channeling in the presence of dislocation loops: New development in the McChasy code", Nucl. Instrum. Method. Phys. Res. Sect. B: Beam Interact. Mater. Atom. 538, 198 (2023)
- [2] P. Jozwik, L. Nowicki, R. Ratajczak, A. Stonert, C. Mieszczyński, A. Turos, K. Morawiec, and K. Lorenz, E. Alves, "Monte Carlo simulations of ion channeling in crystals containing dislocations and randomly displaced atoms", J. Appl. Phys. 126, 195107 (2019)
- [3] E. Kucal, P. Jóźwik, C. Mieszczyński, C. Dufour, and K. Czerski, "Temperature Effects of Nuclear and Electronic Stopping Power on Si and C Radiation Damage in 3C-SiC", Materials 17, 2843 (2024)
- [4] M. Sarwar, R. Ratajczak, C. Mieszczyński, A. Wierzbicka, S. Gieraltowska, R. Heller, S. Eisenwinder, W. Wozniak, E. Guzewicz, "Defect Accumulation in β-Ga<sub>2</sub>O<sub>3</sub> Implanted with Yb", Acta Materialia 268, 119760 (2024)

## Ultrawide-bandgap Ga<sub>2</sub>O<sub>3</sub> - versatile material for power electronics and photonics

F. Guemann<sup>1\*</sup>, K. Hušeková<sup>1</sup>, E. Dobročka<sup>1</sup>, P. Nádaždy<sup>1</sup>, Z. Zápražný<sup>2</sup>, A. Rosová<sup>3</sup>, R. J. Chidambaram<sup>1</sup>, H. Chouhan<sup>1</sup>, J. Keshtar<sup>1</sup>, O. Pohorelec<sup>1</sup>, F. Egyenes<sup>1</sup>, F. Hrubíšák<sup>1</sup>, M. Krettová<sup>1</sup>, S. G. Vadlamudi<sup>1</sup>, I. Kozak<sup>2,4</sup>, A. Kozak<sup>2</sup>, M. Varga<sup>2</sup>, D. Gregušová<sup>1</sup>, A. Laurenčíková<sup>1</sup>, M. Zdurienčík<sup>5</sup>, D. Pudiš<sup>5</sup>, M. Tapajna<sup>2</sup>

1) Institute of Electrical Engineering, Slovak Academy of Sciences, Slovakia

2) Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská cesta 9, 84104 Bratislava, Slovakia

3) Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava, Slovakia

4) V.G. Baryakhtar Institute of Magnetism of the NAS of Ukraine, Acad. Vernadsky Blvd. 36-b, 03142 Kyiv, Ukraine

5) University of Žilina, Slovakia

\* filip.guemann AT savba.sk

Semiconducting gallium oxide (Ga<sub>2</sub>O<sub>3</sub>) is an emerging material with ultrawide bandgap of ~4.7-5.1 eV, high predicted critical electric field > 8 MV/cm, and high transmittance in the ultraviolet region [1-3]. These properties make it a suitable candidate for power-electronic applications, where high voltage/current switching and rectifying is of importance. Ga<sub>2</sub>O<sub>3</sub>-based devices can offer improved power figure-of-merit compared to established wide bandgap materials such as SiC and GaN and providing sufficient technology maturity is reached, they can extend capabilities of these materials and allow for efficient devices for future power conversion applications. While bulk Ga<sub>2</sub>O<sub>3</sub> substrates exist and can be melt-grown by standard techniques such as Czochralski and edge-defined film-fed growth, Ga<sub>2</sub>O<sub>3</sub> heteroepitaxy is often sought as it allows integration with highly-thermally-conductive substrates such as SiC; moderate thermal conductivity and good scalability potential make Si another interesting substrate material. Ga<sub>2</sub>O<sub>3</sub> heteroepitaxy can help to alleviate the excessive device self-heating related to low Ga<sub>2</sub>O<sub>3</sub> thermal conductivity (~11-27 W/mK). Unfortunately, Ga<sub>2</sub>O<sub>3</sub> heteroepitaxy currently offers growth of limited selection of crystal phases and orientations. In case of monoclinic β-Ga<sub>2</sub>O<sub>3</sub>, which represents the only thermally-stable polymorph, heteroepitaxial films typically contain high concentration of defects and rotational variants that contribute to generally much lower crystalline quality, than that typically achieved by homoepitaxy on bulk substrates. Furthermore, heteroepitaxial Ga<sub>2</sub>O<sub>3</sub> films often suffer from low electron mobility and improvements are needed to achieve efficient power-electronic devices. Finally, due to the ultrawide bandgap, Ga<sub>2</sub>O<sub>3</sub> offers applications in the UV optoelectronics and photonics. Solar-blind deep UV photodetectors can find wide range of uses including industrial and home flame detection and UV sanitation for medical facilities. Furthermore, high laser-damage threshold and anisotropic optical properties of Ga<sub>2</sub>O<sub>3</sub> makes it an attractive material for high-power photonics operating in the UV-visible range and can enable photonic integrated circuits for e.g. optical communication and nonlinear optics.

**KEYWORDS:** Gallium oxide, Ga<sub>2</sub>O<sub>3</sub>, Heteroepitaxy, Defects, Power electronics

**ACKNOWLEDGEMENTS:** Funding from Slovak R&D Agency (APVV-24-0325, SK-TW-RD-24-0006), Slovak Grant Agency VEGA (2/0156/25), Slovak Academy of Sciences (CAS-SAS-2024-08, SAS-TUBITAK/JRP/2024/1107.C/COPS) and the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I05-03-V02-00030 is gratefully acknowledged. M.V. acknowledges support from the project IM-2023-87 funded by the Slovak Academy of Sciences via the programme IMPULZ 2023.

### REFERENCES

- [1] S. J. Pearton, *et al.*, A review of Ga<sub>2</sub>O<sub>3</sub> materials, processing, and devices, *Appl. Phys. Rev.* 5, 011301 (2018), <https://doi.org/10.1063/1.5006941>
- [2] S. J. Pearton, *et al.*, Status of Ga<sub>2</sub>O<sub>3</sub> for power device and UV photodetector applications, *Appl. Phys. Rev.* 12, 031336 (2025), <https://doi.org/10.1063/5.0285075>
- [3] M. Q. Li, *et al.*, Highly preferred orientation of Ga<sub>2</sub>O<sub>3</sub> films sputtered on SiC substrates for deep UV photodetector application, *Appl. Surf. Sci.* 471, 694 (2019), <https://doi.org/10.1016/j.apsusc.2018.12.045>

## Subtle structural and optical properties of $\beta$ -Ga<sub>2</sub>O<sub>3</sub> nanolayers: A new frontier in oxide materials

R. Ratajczak<sup>1\*</sup>, J. Matulewicz<sup>1</sup>, E. Grzanka<sup>2</sup>, D. Kalita<sup>1</sup>, M. O. Liedke<sup>3</sup>, S. Prucnal<sup>3</sup>, C. Mieszczynski<sup>1</sup>, P. A. Jóźwik<sup>1</sup>, M. Sarwar<sup>4</sup>, V. Ivanov<sup>4</sup>, E. Guzewicz<sup>4</sup>, W. Woźniak<sup>4</sup>, R. Heller<sup>3</sup>, U. Kentsch<sup>3</sup>, F. Garrido<sup>5</sup>

1) National Centre for Nuclear Research, Otwock, Poland, Poland

2) Institute of High Pressure Physics, Polish Academy of Sciences, Warsaw, Poland, Poland

3) Helmholtz-Zentrum Dresden Rossendorf, Germany

4) Institute of Physics Polish Academy of Sciences, Poland

5) Université Paris-Saclay, CNRS/IN2P3, IJCLab, Orsay, 91405, France, France

\* renata.ratajczak AT ncbj.gov.pl

Rare-earth (RE)-doped  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> nanolayers are promising systems for a new generation of radiation-resistant optoelectronic applications. RE doping extends the optical functionality of this ultrawide-bandgap host material from the ultraviolet into the visible and infrared spectral range, making  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>:RE systems attractive for applications such as phosphors, displays, high-power LEDs, and advanced photodetectors.

Our recent studies have focused on subtle structural and optical changes induced by RE ion implantation in  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> with different crystallographic orientations. Special attention has been given to orientation-dependent defect formation and phase transitions, as well as to the role of rare-earth dopants both as sensitive probes of these processes and as active luminescent centers.

The presentation will address the influence of irradiation-induced defects, structural disorder, and thermal annealing on both the host material and rare-earth emission. To achieve a comprehensive understanding of these processes, we employed a combination of complementary analytical techniques, including positron annihilation spectroscopy (PAS), high-resolution X-ray diffraction (HRXRD), high-resolution transmission electron microscopy (HRTEM), and Rutherford Backscattering Spectrometry in channeling mode (RBS/c), supported by Monte Carlo simulations using the McChasy code [1]. The optical response of RE ions was investigated by photoluminescence (PL). Different rare-earth dopants were investigated to demonstrate how irradiation-induced nanoscale structural transformations, including defect formation [2], phase transitions [3], and their evolution during post-implantation annealing [2-3], affect luminescence efficiency, and excitation mechanisms of RE ions [4]. Our results reveal complex defect accumulation processes in RE-ion-implanted  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>, leading to the formation of both crystalline  $\gamma$ -Ga<sub>2</sub>O<sub>3</sub> and amorphous regions in distinct damage zones. Although these radiation-induced phases disappear after annealing [2-3], complete defect removal is not achieved. Instead, thermal treatment promotes the rearrangement of residual defects into larger defect complexes.

Particular focus has been placed on optimizing implantation and annealing conditions [4-5] to enhance rare-earth luminescence, control defect-related processes, and understand concentration quenching effects. By correlating radiation-induced structural changes with optical functionality through a comprehensive experimental approach, this work highlights RE-doped  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> nanolayers as a new frontier in oxide nanomaterials for tunable light-emitting systems, radiation-tolerant photonics, and advanced optoelectronic devices.

---

**KEYWORDS:** Rare-earth ions, Ion implantation, Radiation damage, Optical activation, Radiation-hard optoelectronics

---

**ACKNOWLEDGEMENTS:** This research was carried out under the NCN project UMO-2022/45/B/ST5/02810 supported by Helmholtz Zentrum Dresden Rossendorf e. V., a member of the Helmholtz Association. We would like to express our gratitude to the IBC and ELBE facility staff for their assistance.

---

### REFERENCES

- [1] P. Jóźwik, A. Caçador, K. Lorenz, R. Ratajczak, and C. Mieszczynski, “Monte Carlo simulations of ion channeling in the presence of dislocation loops: New development in the McChasy code,” Nucl. Instrum. Methods Phys. Res. B, vol. 538, p. 198, 2023.
- [2] M. Sarwar, R. Ratajczak, C. Mieszczynski, A. Wierzbicka, S. Gierałowska, R. Heller, S. Eisenwinder, W. Woźniak, and E. Guzewicz, “Defect accumulation in  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> implanted with Yb,” Acta Mater., vol. 268, p. 119760, 2024.
- [3] R. Ratajczak, M. Sarwar, D. Kalita, P. Jóźwik, C. Mieszczynski, J. Matulewicz, M. Wilczopolska, W. Woźniak, U. Kentsch, R. Heller, and E. Guzewicz, “Anisotropy of radiation-induced defects in Yb-implanted  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>,” Sci. Rep., vol. 14, p. 24800, 2024.
- [4] R. Ratajczak, J. Matulewicz, S. Prucnal, M. O. Liedke, C. Mieszczynski, P. Jóźwik, U. Kentsch, R. Heller, E. Hirschmann, A. Wagner, W. Woźniak, F. Garrido, and E. Guzewicz, “Structural and optical characteristics of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> implanted with rare-earth ions,” arXiv, arXiv:2603.10223, 2026.
- [5] M. Sarwar, R. Ratajczak, V. Ivanov, S. Gierałowska, A. Wierzbicka, W. Woźniak, R. Heller, S. Eisenwinder, and E. Guzewicz, “Crystal lattice recovery and optical activation of Yb implanted into  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>,” Materials, vol. 17, p. 3979, 2024.

## Multilayer gap plasmons

A. Pinchuk<sup>1</sup> \*

*1) Department of Physics and Energy Science, University of Colorado Colorado Springs, USA*

\* apinchuk AT uccs.edu

Gap plasmons provide strong electromagnetic field confinement and enhanced propagation compared with conventional surface plasmon polaritons. While single gap plasmon modes have been extensively studied, multilayer gap plasmon systems remain largely unexplored. Theoretical and computational investigation of multilayer plasmonic systems is important because coupling between layers can enable additional control over propagation characteristics, dispersion behavior, and field localization.

This work introduces multilayer gap plasmons supported by alternating metallic and dielectric layers containing periodic subwavelength slits [1]. The study demonstrates that collective plasmon modes can propagate through the entire multilayer stack, enabling new degrees of freedom for waveguiding, metasurface design, and metamaterial engineering.

The results demonstrate that multilayer structures support multiple propagating gap plasmon modes across the full stack thickness. As the number of layers increases, the number of supported modes increases and approaches a continuous band structure in the infinite-layer limit. [1]

The calculated wave number spectrum extends both below and above the free-space wave number. Modes below the free-space wave number correspond to leaky or weakly confined modes that become more confined as layer number increases, while higher wave number modes exhibit strong confinement and enhanced interlayer coherence.

Field profile analysis confirms that electromagnetic energy is localized primarily within dielectric gap regions, while metallic regions remain field-free except within slit openings. Higher-order spatial harmonics introduce only minor phase shifts without significantly distorting mode shape, confirming that the fundamental mode dominates propagation behavior.

---

**KEYWORDS:** Gap plasmons, Multilayer gap plasmon, Periodic subwavelength slits

---

**ACKNOWLEDGEMENTS:** We acknowledge partial support from NATO-SPS - G6197 grant.

---

### REFERENCES

- [1] M. Haftel, J. Case, and Anatoliy Pinchuk, “Multilayer gap plasmons” *Optical Materials Express*, Vol. 15, 9, pp. 2164-2174, (2025)

## Analytical model of Raman gain dynamics in singlemode telecommunication fibers with multiwave pumping

V. Zaika<sup>1</sup>\*, G. Felinskyi<sup>1</sup>, V. Grygoruk<sup>1</sup>, S. Felinskyi<sup>1</sup>, I. Serdeha<sup>1</sup>

1) Institute of High Technologies, Taras Shevchenko National University of Kyiv, Ukraine

\* vlad40426 AT gmail.com

Raman nanophotonics is part of the high technologies that provide record speeds of information exchange [1] in fiber optic telecommunication systems. Modern fiber lasers and optical amplifiers based on nonlinear light amplification by the stimulated Raman effect [2] are widely used in global telecommunications with terabit bandwidth. The widespread use of nonlinear photonics in modern telecommunications is explained by the simplicity of technical implementation of nonlinear light amplification devices [3] to ensure terabit speed information exchange systems [4]. However, device modeling encounters the great complexity of fundamental processes involving the interaction between many optical signal and pump waves under the influence of molecular nanocomplexes in the optical fiber core. A significant number of modeling techniques have been proposed over the past two decades, ranging from direct numerical solutions of systems of hundreds of differential equations [5] to a large number of alternative phenomenological approaches based on metaheuristic algorithms [6]. Regression models such as Linear Regression (LR), Random Forest (RF), Support Vector Regression (SVR), Gradient Boosting (GB), Artificial Neural Networks (ANNs), and/or improved whale algorithms [7] must first be trained and tested on the basis of statistical performance measures. Therefore, the modeling problem of Raman gain dynamics in single mode telecommunication fibers remains a subject of intensive research. Furthermore, if the properties of the Raman effect are taken into account in more detail, device modeling requires innovative approaches free from the limitations imposed by the numerical methods listed above [8]. Our work presents a quantitative criterion for the nominal operating mode of the FRA without self excitation in the form of the critical signal power at the output of the nonlinear amplifier. On this basis, the applicability of the weak signal model for analyzing Raman gain dynamics in single mode telecommunication fibers with multiwavelength pumping has been proven. The suitability of our model is confirmed by test calculations for standard single mode fibers based on silica glass, namely DCF and TrueWave RS types. The Raman gain profiles of these fibers are given in analytical form. The results of a comparative analysis of distributed FRA parameters designed to operate in several telecommunication fiber transparency windows are presented. The advantages of the analytical model over other methods related to the direct solution of complex systems of differential equations are discussed.

**KEYWORDS:** Raman scattering, Nonlinear photonics, Telecommunication systems, Optical fiber, DCF

### REFERENCES

- [1] B. J. Puttnam, *et al.*, "1 Pb/s Transmission in a 125 $\mu$ m diameter 4-core MCF," 2022 Conference on Lasers and Electro-Optics (CLEO), San Jose, CA, USA, 2022, pp. 1-2. <https://www.nict.go.jp/en/press/2022/05/30-1.html>
- [2] L. Sirleto, M.A. Ferrara. Fiber amplifiers and fiber lasers based on stimulated Raman scattering: A Review. *Micromachines*, 2020, 11(3), 247; <https://doi.org/10.3390/mi11030247>.
- [3] L. Galdino *et al.*, "Amplification Schemes and Multi-Channel DBP for Unrepeated Transmission," *J. Lightwave Techn.*, 2016, 34(9), pp. 2221-2227, 1 May1, doi: 10.1109/JLT.2016.2521002.
- [4] M.N. Islam. Raman amplifiers for telecommunications // *IEEE J. Sel. Top. Quant. Electron.* - 2002. - Vol. 8, N 3. - P. 548-559.
- [5] H. Kidorf *et al.*, "Pump interactions in a 100-nm bandwidth Raman amplifier," in *IEEE Photonics Technology Letters*, vol. 11, no. 5, pp. 530-532, May 1999, doi: 10.1109/68.759388.
- [6] F. Qamar, M. Islam, R. Shahzadi, A. Shahzad, N. Qamar. Comparative analysis of ML algorithms for the design of intelligent EDFA. *Journal of Optical Communications*. <https://doi.org/10.1515/joc-2026-0037>
- [7] J. Yao and H. Deng. "Fiber Raman Amplifier Based on Improved Whale Algorithm" The 2nd International Conference on Electronic Information and Communication Engineering (EICE 2023) 13- 15 Jan 2022 Guangzhou, China, *J. Phys.: Conf. Ser.* 2525 012016, 2023 DOI: 10.1088/1742- 6596/2525/1/012016
- [8] V. Zaika, V. Grygoruk and G. Felinskyi, "Modeling of Multiwaves Pumped Raman Amplification in DCF Type Silica Fiber with Minimal Gainband Ripples Within C+L Telecommunication Windows," 2025 IEEE 15th Int. Conf. Nanomaterials: Applications & Properties (NAP), Bratislava, Slovakia, 2025, pp. UBMP021-UBMP024, <https://doi.org/10.1109/NAP68437.2025.11216222>

## Effect of dopant nature on luminescence and phase stability of rare-earth doped zirconia

L. Khomenkova<sup>1,2\*</sup>, K. Kozoriz<sup>1</sup>, N. Korsunska<sup>1</sup>, L. Borkovska<sup>1</sup>, V. Khomenkov<sup>3</sup>, Y. Brodnikovskiy<sup>4</sup>,  
O. Melnichuk<sup>5</sup>, L. Melnichuk<sup>5</sup>, Y. Smortsova<sup>6</sup>, O. Chukova<sup>6</sup>, X. Portier<sup>7</sup>, F. Goubilleau<sup>7</sup>

1) V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine, Ukraine

2) National University "Kyiv-Mohyla Academy", Ukraine

3) Institute for Nuclear Research, NAS of Ukraine, Ukraine

4) Frantsevich Institute for Problems of Materials Science, 3 Krzhizhanovskiy Str., Kyiv, 03860, Ukraine, Ukraine

5) Mykola Gogol State University of Nizhyn, 2 Hrafska str., Nizhyn 16600, Ukraine, Ukraine

6) Deutsches Elektronen Synchrotron DESY, Germany

7) CIMAP, CEA, UMR CNRS 6252, ENSICAEN, Normandie Université, 14000 Caen, France, France

\* khomen AT ukr.net

Zirconia ( $ZrO_2$ ) is a widely used functional oxide due to its high chemical stability, favorable dielectric properties, and tunable defect structure. Its phase stability and functional response are strongly influenced by dopant type and concentration, which govern the formation of oxygen vacancies, grain size evolution, and polymorphic transformations. Understanding dopant-lattice interactions is therefore essential for the design of advanced oxide materials.

In this work, structural and optical properties of  $ZrO_2$  nanopowders and ceramics doped and co-doped with rare-earth ions were investigated as a function of composition and processing conditions using UV-vis diffuse reflectance, synchrotron-based excitation-emission photoluminescence mapping, scanning electron microscopy, X-ray diffraction, Raman scattering, FTIR and energy-dispersive spectroscopy.

It was found that phase stability is highly sensitive to dopant combinations and processing parameters. Single doping (e.g.,  $Yb^{3+}$  or  $Eu^{3+}$ ) leads to stabilization of the cubic phase, while in co-doped systems (e.g., Sc-Ce) additional incorporation of Gd is required to suppress the formation of secondary rhombohedral phases. The Ce/Gd ratio was identified as a key factor controlling cubic phase stability. Thermal processing conditions, including heating rate and sintering time, were shown to significantly influence microstructure evolution by reducing porosity and inhibiting undesired phase transformations.

Taking into account the strong sensitivity of rare-earth luminescence to local symmetry, photoluminescence excitation-emission maps enabled identification of different structural environments and contributions from coexisting polymorphs. The obtained results provide insight into excitation pathways and allow discrimination between host-related and dopant-related emission.

The combined structural and optical analysis demonstrates that precise control of dopant chemistry and thermal processing enables tuning of phase composition, defect structure, and luminescent properties of zirconia-based materials, offering promising approaches for the development of functional ceramics for photonic and energy-related applications.

**KEYWORDS:**  $ZrO_2$  nanopowders, Ceramics, Rare-earth doping, Phase stability, Luminescence

**ACKNOWLEDGEMENTS:** This work was supported by the National Academy of Sciences of Ukraine through the R&D Grant No. 0125U000995 “Development of material technology, circuit design solutions, and the structural design of a modular solar charging device”, funded under the Ukrainian State Budget Program “Support for the Development of Priority Scientific Research Directions” for 2025-2026. This project has also received funding from the European Union’s Horizon 2020 research and innovation programme under Grant Agreement No. 101007417 and the authors acknowledge access to the P66 beamline at PETRA III, DESY (Hamburg, Germany), within the framework of the NFFA-Europe Pilot Transnational Access activity (proposal ID 865). The authors (L.K., L.B., V.K.) are grateful to the DESY User Office for financial support provided through the NEPHEWS project funded by the Horizon Europe programme (proposals I-20240812 EC and I-20250701 EC).

## Upconversion luminescence from Er-Yb-Bi codoped clinoptilolite

V. Vasylechko<sup>1</sup>, L. Shevchuk<sup>2\*</sup>, O. Kostiv<sup>2</sup>, R. Gamernyk<sup>2</sup>, A. Voloshinovskii<sup>2</sup>, O. Gromyko<sup>2</sup>, S. Bagday<sup>2</sup>

1) Ivan Franko National University of Lviv, Lviv University of Trade and Economics, Ukraine

2) Ivan Franko National University of Lviv, Ukraine

\* liubomyr.shevchuk AT lnu.edu.ua

Zeolites are promising materials for the creation of new materials with optically active centres, as their structure contains Si-O-Al and Si-O-Si groups with low-energy vibrations, and their pores can be used to accommodate cations, in particular rare earth elements. There are luminophores based on synthetic zeolites doped with lanthanides, which operate via an upconversion mechanism in which lower-energy light is converted into higher-energy light through multiphoton absorption and energy transfer processes. Compared to low-conversion luminescent (LM) materials, LM upconversion labels demonstrate intriguing advantages, such as very low background light, high penetration depth, high detection sensitivity and low photodamage to biological samples. The most effective upconversion LM materials are based on the Er<sub>3+</sub> ion in combination with the Yb<sub>3+</sub> ion as a sensibiliser, which exhibits green and red emission. The presence of Bi can enhance the efficiency of the upconversion luminophore, as this metal can act as an excellent material for blocking and sealing zeolite pores, thereby protecting the optically active centres from LM quenching. A natural zeolite-containing mineral from the deposit in the village of Sokirnytsia in the Ukrainian Transcarpathian region was used in the current study. Transcarpathian clinoptilolite (CL) is an effective sorbent for rare earth elements. During the synthesis of upconversion LM materials based on the “CL-Bi(III)-Er(III)-Yb(III)” composition, the results of studies on the sorption properties of CL with respect to Yb(III), Er(III), and Bi(III) were utilised. A Yb laser with a power of 3 W ( $\lambda = 980$  nm) was used to excite the upconversion LM. In the upconversion LM spectra of samples based on Transcarpathian CL, in addition to the peaks at  $\lambda = 633$  nm and 539 nm, which correspond to red and green emission, two further peaks are clearly visible at  $\lambda = 492$  nm and  $\lambda = 380$  nm. Moreover, the highest LM intensity is observed at  $\lambda = 492$  nm. The LM intensity at  $\lambda = 380$  nm is minimal for samples that do not contain Yb. The absolute Yb content is of key importance for LM in this spectral region. At  $\lambda = 492$  nm, the intensity of samples without Bi is very high; however, with equal Er and Yb contents, the presence of Bi enhances the LM. The Yb content in the samples has virtually no effect on the LM intensity at  $\lambda = 539$  nm. The efficiency of green emission increases with an increase in the Yb/Er ratio. The intensity of LM at  $\lambda = 633$  nm is even slightly reduced if the samples contain Bi. An increase in the Er content in the samples leads to a decrease in the intensity of red emission. The upconversion LM materials we have synthesised and investigated can be used as quantum dot-labelled nanoparticles in vitro cell cultures. Upon irradiation of such biomaterials, they degrade much more slowly than their organic counterparts, i.e. they possess high photostability. Furthermore, they exhibit low overall toxicity to living organisms.

**KEYWORDS:** Clinoptilolite, Er-Yb-Bi codoped clinoptilolite, Upconversion luminescence

**ACKNOWLEDGEMENTS:** This work partially funded by the Ministry of Education and Sciences of Ukraine.

## Peculiarities of the growth mechanism in ultrathin amorphous $\text{MoSi}_{1-x}$ films

O. O. Leha<sup>1\*</sup>, O. V. Zraichenko<sup>1</sup>, O. G. Turutanov<sup>1</sup>, V. Y. Lyakhno<sup>1</sup>

1) B. Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine, Ukraine

\* leha AT ilt.kharkov.ua

Amorphous superconducting MoSi thin films are promising materials for applications in superconducting nanoelectronics, especially for single-photon detection (SNSPD) in the infrared spectral range, where conventional photon counters lose efficiency [1]. Their electrical and superconducting properties are strongly governed by growth conditions, structural homogeneity, and level of disorder [2].

However, questions remain regarding how deposition parameters influence structural properties and, consequently, superconducting behavior. Here we present a systematic investigation of the growth of MoSi thin films deposited by DC magnetron sputtering from two separate sources in an argon atmosphere for films with various thicknesses down to 1 nm. The influence of discharge power, stoichiometry, and substrate material on film thickness, density, and composition was analyzed using XRR and XPS.

We show that variation of deposition parameters can lead to changes in film composition, as revealed by XPS analysis, alongside modifications in structural characteristics identified by XRR. Compared to previously assumed homogeneous amorphous behavior, our results reveal that even subtle structural variations significantly affect charge transport [3]. We demonstrate that the sheet resistance  $R_s$  systematically varies with deposition parameters, as determined by four-probe measurements. Disorder-induced localization contributes to variations in normal-state sheet resistance  $R_s$  of the film down to 1 nm thick and broadening of the superconducting transition as was observed. Additionally, correlations between composition, density, and thickness obtained from XRR/XPS analysis provide deeper insight into growth-driven structural evolution. These findings establish a direct link between deposition conditions, structural characteristics, and superconducting performance. They provide a basis for optimizing the fabrication of MoSi thin films with tailored properties for next-generation superconducting nanoelectronic devices, including single-photon detectors.

---

**KEYWORDS:** MoSi thin films, DC magnetron sputtering, XRR, XPS, AFM

---

**ACKNOWLEDGEMENTS:** This work is supported by the National Research Foundation of Ukraine, project No.22.07/0044 and by the IEEE program “Magnetism for Ukraine 2025-2026”, project number 9918.

---

### REFERENCES

- [1] Yu. P. Korneeva, M. Yu. Mikhailov, Yu. P. Pershin, N. N. Manova, A. V. Divochiy, Yu. B. Vakhtomin, A. A. Korneev, K. V. Smirnov, A. G. Sivakov, A. Yu. Devizenko, G. N. Goltsman., “Superconducting single-photon detector made of MoSi film”, *Superconductor Science and Technology*, 27(9), 095012 (2014).
- [2] S. Grotowski, L. Zugliani, B. Jonas, R. Flaschmann, C. Schmid, S. Strohauser, F. Wietschorke, N. Bruckmoser, M. Müller, M. Althammer, R. Gross, K. Müller, J. Finley, “Optimizing the growth conditions of superconducting MoSi thin films for single photon detection”, *Sci. Rep.*, 15, 2438 (2025).
- [3] Z. Liu, B. Luo, J. Hu, C. Xing, "Transport mechanism in amorphous molybdenum silicide thin films", *Journal of Physics and Chemistry of Solids*, 149, 109818 (2021).

# Track 7

Magnetic Materials, Magnonics and Spin Phenomena

## Atomic scale Structure-Function correlations in spintronic nanomaterials and heterostructures

V. K. Lazarov<sup>1,2,\*</sup>, J. A. D. Nascimento<sup>1</sup>, B. Achinuq<sup>1</sup>, Z. Nedelkoski<sup>3</sup>, L. Lari<sup>1,2</sup>, A. Kerrigan<sup>1,2</sup>,  
Q. Ramasse<sup>4</sup>, D. M. Kepaptsoglou<sup>1,4</sup>, S. Majetich<sup>5</sup>, R. F. L. Evans<sup>1</sup>, L. Li<sup>6</sup>, M. Weinert<sup>6</sup>, K. Hamaya<sup>7</sup>

1) School of PET, University of York, York YO10 5DD, United Kingdom

2) York-JEOL Nanocentre, University of York, York, YO10 5BR, United Kingdom

3) Faculty of Technical Sciences, University Mother Theresa, Skopje 1000 (Macedonia (The former Yugoslav Republic of))

4) SuperSTEM Laboratory, SciTech Daresbury Campus, Daresbury WA4 4AD, United Kingdom

5) Physics Department, Carnegie Mellon University, Pittsburgh, PA 15213, USA

6) Department of Physics, University of Wisconsin-Milwaukee, Milwaukee, WI 53211, USA

7) Graduate School of Engineering Science, Osaka University, Osaka, 560-8531, Japan

\* vlado.lazarov AT york.ac.uk

Spintronics has attracted significant attention over the past two decades due to its potential to revolutionize CMOS-based logic and data devices through the utilisation of electron spin. Spin manipulation via spin current generation, propagation, as well as spin injection and detection, represents key steps toward the realization of fast, non-volatile, and increasingly important low-power computational devices. Achieving these goals remains highly challenging, requiring atomic-level control of interfaces and thin-film structures in multilayered heterostructures composed of ferromagnetic and antiferromagnetic alloys and oxides, semiconductor layers, half-metals, and topological insulators.

In this work, utilising advanced electron microscopy techniques such as Scanning Transmission Electron Microscopy (STEM), Electron Energy Loss Spectroscopy (EELS), Energy Dispersive X-ray Spectroscopy (EDX), as well as Scanning Tunnelling Microscopy and Spectroscopy (STM/STS), we present an overview of the correlation between atomic structure and functionality in nanoparticles, thin films, and heterostructures. Particular emphasis is placed on the role of inhomogeneities, including interfaces, grain boundaries, point defects, and strain, in determining magnetic properties, spin dynamics, and spin-device performance. First, we discuss how atomic chemical ordering influences magnetotransport properties of magnetite nanoparticles and thin films of Fe<sub>3</sub>O<sub>4</sub>, as well as heterostructures of half-metallic Co-based Heusler alloys with Si and Ge, aiming to achieve near 100% spin polarization in thin films. Control of half-metal/semiconductor interfaces for maximising spin injection is also addressed. The second part focuses on the role of strain in controlling topological states in the Bi<sub>2</sub>Se<sub>3</sub> three-dimensional topological insulator, where tensile strain induces a band gap at the topologically protected surface states. Finally, we discuss the recent demonstration of detecting spin-wave excitations (magnons) using low-energy momentum-resolved EELS in ferromagnetic and antiferromagnetic materials [1-3], along with prospects for atomic-scale imaging of spin structures.

---

**KEYWORDS:** STEM, EELS, Spintronics, Halfmetals, Magnons

---

**ACKNOWLEDGEMENTS:** We thank Engineering and Physical Sciences Research Council (EPSRC) funding via following research grants: EP/Z531194/1, EP/W021080/1, EP/S033394/1.

---

### REFERENCES

- [1] Kepaptsoglou *et al.* Nature 644 (8075), 83 (2025)
- [2] do Nascimento *et al.*, New Journal of Physics 27 (11), 113505 (2025)
- [3] do Nascimento *et al.* Physical Review B 110 (2), 024410 (2025).

## The hidden universality in charge/spin current interconversion and magnetoresistance

X. Wang<sup>1</sup>\*

1) The Chinese University of Hong Kong (Shenzhen), China

\* phxwan AT cuhk.edu.cn

The universal features for charge/spin current interconversion involved tensor order parameters and for magnetoresistance controlled by two vectors in magnetic multilayers are predicted [1-4]. The universal featured termed as anomalous spin-Hall effect and anomalous inverse spin-Hall effect exists are confirmed by recent experiments [5-6]. The universal anisotropic magnetoresistance (UAMR) and unidirectional magnetoresistance (UMR) observed in all nanoscale bilayers or multilayers [7-8] can naturally arise from electron transport influenced by the magnetization vector present in the magnetic material and the interfacial potential inherent in heterostructures [6-8]. Specifically, UAMR represents current-independent resistance (resistivity) in bilayers, while UMR is characterized by resistance that is proportional to the current, even though electron transport in the bilayers is a linear response to high current densities and the induced thermal gradients [4]. The predictions of our theory align well with existing experimental results [7] and with observations in layered Van der Waals magnetic films [8] and have also been confirmed by first-principles calculations [9]. Furthermore, this framework offers a universal perspective that not only bridges UMR and UAMR effects, enhancing our understanding of spin-dependent transport phenomena in bilayers, but also provides a unified picture for well-known MR phenomena: the usual AMR in polycrystalline ferromagnets as a consequence of one-vector physics, and AMR in ferromagnetic single crystals as a consequence of four-vector physics [10].

**KEYWORDS:** Anomalous spin-Hall and inverse spin-Hall effect, Unusual anisotropic magnetoresistance, Unidirectional magnetoresistance, Magnetic bilayers, And multilayers

**ACKNOWLEDGEMENTS:** This work is supported by the NSFC Grant (No. 12374122), the Guangdong Provincial Quantum Strategy Special Project, and the University Development Fund of the Chinese University of Hong Kong, Shenzhen

### REFERENCES

- [1] Anomalous spin Hall and inverse spin Hall effects in magnetic systems”, X. R. Wang, *Commun. Phys.* 4, 55 (2021).
- [2] A theory of unusual anisotropic magnetoresistance in bilayer heterostructures”, X. R. Wang, C. Wang, and X. S. Wang *Scientific Reports* 13, 309 (2023).
- [3] A Theory for Anisotropic Magnetoresistance in Materials with Two Vector Order Parameters”, X. R. Wang, *Chinese Physics Letters* 39(2) 027301 (2022).
- [4] Unified theory of anisotropic magnetoresistance and unidirectional magnetoresistance in nanoscale bilayers”, X. R. Wang, *Phys. Rev. B* 112, 094451 (2025).
- [5] Anomalous inverse spin Hall effect in perpendicularly magnetized Co/Pd multilayers”, M. Yang, B. Miao, J. Cheng, K. He, X. Yang, Y. Zeng, Z. Wang, L. Sun, X. R. Wang, A. Azevedo, S. Bedanta, and H. Ding, *Phys. Rev. B* 105, 224426 (2022).
- [6] Highly efficient field-free switching of perpendicular yttrium iron garnet with collinear spin current”, M. Yang, L. Sun, Y. Zeng, J. Cheng, K. He, X. Yang, Z. Wang, L. Yu, H. Niu, T. Ji, G. Chen, B. Miao, X. R. Wang, and H. Ding, *Nat. Commun.* 15, 3201 (2024).
- [7] Physics Origin of Universal Unusual Magnetoresistance”, L. Zhu, Q. Liu, X. R. Wang, *National Science Review* 12, nwaf240 (2025).
- [8] Unusual Van der Waals Magnetoresistance in Stacked Ferromagnetic Fe<sub>3</sub>GeTe<sub>2</sub>: The Role of Atomically Sharp Interfaces”, Q. Chen, J. Sun, J. Liang, W. Jiang, Z. Yu, Z. Zeng, Y. Zhai, K. Xia, and X. R. Wang, *Advanced Science* e08244 (2025).
- [9] Anisotropic magnetoresistance due to magnetization-dependent spin-orbit in teractions”, M. Q. Dong, Zhi-Xin Guo, and X. R. Wang, *Phys. Rev. B* 108, L020401 (2023).
- [10] Anisotropy galvanomagnetic effects in single cubic crystals: A theory and its verification”, Y. Miao, J. Sun, C. Gao, D. S. Xue, and X. R. Wang, *Phys. Rev. Lett.* 132, 206701 (2024).

## Magnetic time-varying metamaterials

S. Tomita<sup>1\*</sup>

1) Tohoku University, Japan

\* tomita AT tohoku.ac.jp

Metamaterials are man-made structured materials exhibiting intriguing optical properties unavailable in natural materials. The most typical examples are metamaterials for negative refractive indices and for invisible cloaks. These are referred to as space-varying metamaterials because of the spatially modulated refractive indices. Very recently, a new paradigm for light generation and steering using metamaterials has emerged - time-varying metamaterials, in which refractive indices are temporally modulated. Time-varying metamaterials bring about exotic phenomena, for example, time refraction, time reflection, and analogue of a continuous time crystal as well as promising applications to frequency converters and nonreciprocal devices. Furthermore, time-varying metamaterials mimic magnetoelectric interaction in equivalent moving media [1]. However, experimental demonstration of time modulation in magnetic permeability is still lacking [2,3] while time-varying electric permittivity has been achieved. Therefore, time-varying permeability metamaterials are highly desired. In this talk, we demonstrate magnetic time-varying metamaterials using ferromagnetic resonance at GHz frequencies in magnetic permalloy ( $\text{Ni}_{80}\text{Fe}_{20}$ ) thin films. The experimental results are reproduced via numerical simulation, verifying that frequency conversion observed is caused by time modulation of magnetic permeability [4]. The present study opens a door to magnetoelectric metamaterials with synthetic motion for probing quantum vacuum effects.

---

**KEYWORDS:** Metamaterial, Magnetic permeability, Ferromagnetic resonance

---

**ACKNOWLEDGEMENTS:** This work is financially supported by JST-CREST (JPMJCR2102) and JSPS-KAKENHI (A24H022320, 25K00929).

---

### REFERENCES

- [1] P. A. Huidobro *et al.*, PNAS 116, 24943 (2019).
- [2] T. Kodama *et al.*, Physical Review Applied 19, 044080 (2023).
- [3] T. Kodama *et al.*, Physical Review B 109, 214419, (2024).
- [4] T. Kodama *et al.*, arXiv:2503.04571.

## Grain boundary engineering of Sm(Fe-Co)-B hard magnetic thin films

T. Shima<sup>1</sup>\*

*1) Tohoku Gakuin University, Japan*

\* shima AT mail.tohoku-gakuin.ac.jp

RFe<sub>12</sub>(R: rare earth) compounds with the ThMn<sub>12</sub>-type structure are promising candidates for next-generation permanent magnets due to their high saturation magnetization and anisotropy field with reduced rare-earth content. Epitaxial Sm(Fe<sub>0.8</sub>Co<sub>0.2</sub>)<sub>12</sub> thin films have demonstrated excellent magnetic properties, including  $\mu_0 M_s = 1.78$  T,  $\mu_0 H_a = 12$  T, and  $T_C = 859$  K [1]. In B-doped Sm(Fe-Co)<sub>12</sub>-B thin films, we previously achieved a coercivity of 1.2 T by forming a columnar structure where SmFe<sub>12</sub> grains are surrounded by a B-rich amorphous grain boundary phase [2]. Furthermore, micromagnetic studies predicted that coercivity could reach ~6 T if the  $\alpha$ -(Fe,Co) phase at the interface between the V underlayer and the magnetic layer is suppressed [3]. In this study, microstructural control was performed to further enhance magnetic properties by introducing a Sm seed layer and applying post-annealing to promote cap layer diffusion. Thin films were fabricated using ultra-high vacuum magnetron sputtering. A V buffer layer and Sm seed layer were deposited on MgO (100) substrates at 400 °C, followed by the Sm(Fe-Co)-B layer. Structural and magnetic properties were characterized by XRD, SEM, AFM, and SQUID. XRD results showed that introducing the Sm seed layer reduced  $\alpha$ -(Fe,Co) phase formation and enhanced (002) and (004) peaks of the ThMn<sub>12</sub> phase. Magnetization curves revealed suppression of low-field soft magnetic contributions. Consequently, Sm/Sm(Fe,Co)<sub>12</sub>-B films exhibited improved remanence while maintaining coercivity above 1.0 T. These results indicate that the Sm seed layer effectively suppresses soft phase formation and improves crystallographic orientation, highlighting the importance of microstructural control in enhancing coercivity.

---

**KEYWORDS:** Permanent magnet, ThMn 12 -type structure, Thin film, Coercivity, Grain boundary

---

**ACKNOWLEDGEMENTS:** This work was performed at the research Institute for Engineering and Technology at Tohoku Gakuin University. This work was partly supported by the MEXT program: Data Creation and Utilization-Type Material Research and Development Project (Digital Transformation Initiative Center for Magnetic Materials) Grant Number JPMXP1122715503.

---

### REFERENCES

- [1] Y. Hirayama, Y. K. Takahashi, S. Hirose and K. Hono, “Intrinsic hard magnetic properties of Sm(Fe<sub>1-x</sub>Co<sub>x</sub>)<sub>12</sub> compound with the ThMn<sub>12</sub> structure”, *Ser. Mater.*, 138, 62 (2017).
- [2] H. Sepeshri-Amin, Y. Tamazawa, M. Kambayashi, G. Saito, Y. K. Takahashi, D. Ogawa, T. Ohkubo, S. Hirose, M. Doi, T. Shima and K. Hono, “Achievement of high coercivity in Sm(Fe<sub>0.8</sub>Co<sub>0.2</sub>)<sub>12</sub> anisotropic magnetic thin film by boron doping”, *Acta Mater.*, 194, 337-342 (2020).
- [3] A. Boyachkin, H. Sepeshri-Amin, M. Kambayashi, Y. Mori, T. Ohkubo, Y. K. Takahashi, T. Shima and K. Hono, "Coercivity engineering in Sm(Fe<sub>0.8</sub>Co<sub>0.2</sub>)<sub>12</sub>B<sub>0.5</sub> thin films by Si grain boundary diffusion", *Acta. Mater.*, 227(2022) 117716.
- [4] J. Uzuhashi, Y. Mori, T. Koyama, T. Abe, Y. K. Takahashi, T. Shima, "Grain-boundary engineering of Sm(FeCo)<sub>12</sub>-B thin films via boron absorption", *Acta Mater.*, 309(2026)122098.

## Demagnetization process and magnetic properties of CeZrFe<sub>11</sub>/FeCo nanocomposite grains

K. Koike<sup>1\*</sup>, A. Kobayashi<sup>1</sup>, Y. Mano<sup>1</sup>, M. Nakano<sup>2</sup>, M. Itakura<sup>3</sup>, S. Okubo<sup>4</sup>

1) Department of Applied Mathematics and Physics, Graduate School of Science and Engineering, Yamagata University, Japan

2) Graduate School of Integrated Science and Technology, Nagasaki University, Japan

3) Department of Advanced Materials Science and Engineering, Kyushu University, Japan

4) Molecular Photoscience Research Center, Kobe University, Japan

\* kkoike AT yz.yamagata-u.ac.jp

Permanent magnets with reduced use of critical rare-earth elements are strongly required for sustainable energy technologies. ThMn<sub>12</sub>-type CeZrFe<sub>11</sub> is a promising hard magnetic material because of its high Curie temperature, large uniaxial magnetocrystalline anisotropy, and the abundance and low cost of Ce [1]. However, its saturation magnetization is relatively low, which limits the maximum energy product. Exchange coupling with a soft magnetic phase having high saturation magnetization is therefore expected to improve the magnetic performance [2, 3]. However, the effects of laminated nanostructure and grain arrangement on the demagnetization process of CeZrFe<sub>11</sub>-based nanocomposite grains have not been sufficiently clarified.

Here, we show the demagnetization process and magnetic properties of exchange-coupled CeZrFe<sub>11</sub>/FeCo laminated nanocomposite grains by micromagnetic simulations using MuMax<sub>3</sub> [4]. In STEP I, single-particle models were examined by changing the FeCo layer thickness and the number of FeCo layers. In STEP II, multi-grain models were also investigated to clarify the effect of grain arrangement, including an inclined structure.

The results showed that the magnetic properties strongly depend on both the laminated structure and the grain arrangement. In the single-grain model, the maximum energy product increased from 250 kJ/m<sup>3</sup> for single-phase CeZrFe<sub>11</sub> to 373 kJ/m<sup>3</sup> for the laminated nanocomposite grains with one FeCo layer, and further reached 742 kJ/m<sup>3</sup> for the optimized structure with four FeCo layers and a layer thickness of 10 nm. In the multi-grain models, the inclined arrangement improved the maximum energy product by about 3% compared with the symmetric arrangement, and the value reached 434 kJ/m<sup>3</sup>.

These results indicate that optimization of the FeCo layer thickness, the number of layers, and the grain arrangement is effective for improving the demagnetization behavior and energy product of CeZrFe<sub>11</sub>-based nanocomposite magnets. This study provides a useful design guideline for high-performance permanent magnets with reduced Ce content by controlling nanocomposite and inclined structures, and is also consistent with our previous studies on hard/soft nanocomposite magnet design and layered hard/soft grain models [5].

---

**KEYWORDS:** CeZrFe 11, FeCo, Nanocomposite magnets, Demagnetization process, Micromagnetic simulation

---

**ACKNOWLEDGEMENTS:** This research has been supported by JSPS KAKENHI, Japan (JP16H04488, JP20K05059, JP20H02425, JP24K08014, JP25K22090).

---

### REFERENCES

- [1] C. Bhandari and D. Paudyal, “First-principles study of ThMn<sub>12</sub>-type CeZrFe<sub>11</sub>,” *Phys. Rev. Res.*, 4, 023013 (2022).
- [2] R. Skomski and J. M. D. Coey, “Giant energy product in nanostructured two-phase magnets,” *Phys. Rev. B*, 48, 15812-15816 (1993).
- [3] R. S. Sundar and S. C. Deevi, “Soft magnetic FeCo alloys: alloy development, processing, and properties,” *Int. Mater. Rev.*, 50, 157-192 (2005).
- [4] A. Vansteenkiste, J. Leliaert, M. Dvornik, M. Helsen, F. Garcia-Sanchez, and B. Van Waeyenberge, “The design and verification of MuMax3,” *AIP Adv.*, 4, 107133 (2014).
- [5] R. Uda, K. Koike, N. Inaba, H. Kato, M. Itakura, S. Okubo, H. Ohta, and H. Tsuchiura, “Maximum energy product of exchange-coupled Sm(FeCo)<sub>12</sub>/α-Fe nanocomposite particle,” *AIP Adv.*, 13, 025311 (2023).

## Nanocrystal alignment impact on static and dynamic magnetic phase transitions

A. Berger<sup>1</sup>\*

1) CIC nanoGUNE, Spain

\* a.berger AT nanogune.eu

Non-equilibrium phase transitions occur across a wide range of physical systems. A relevant example is the dynamic phase transition (DPT) in ferromagnets, for which the time-averaged magnetization  $Q$  has been identified as the dynamic order parameter. Hereby, it has been observed that  $Q$  changes sharply if an oscillating field undergoes changes in its amplitude  $H_0$  or period  $P$ . It has also been documented that  $Q$  is dependent on the presence of an additional time-independent bias field  $H_b$ , which turns out to be the conjugate field of  $Q$  [1]. Studies of the DPT have yielded important insights into dynamically ordered systems, their phase-space behavior, criticality and transient properties, finding strong qualitative similarities in between  $Q$  as a function of  $P$  and  $H_b$  and the thermodynamic magnetic order parameter  $M$  as a function of  $T$  and  $H$  [1,2]. One key difference between thermodynamic and non-equilibrium systems are metamagnetic anomalies in the paramagnetic dynamic state that do not exist in thermodynamic equilibrium [3]. Furthermore, it is noteworthy that all existing studies to date have focused on Ising-type systems, restricting our present understanding to a single material class [4].

In our study here, we experimentally investigate the DPT in polycrystalline Co films that exhibit very weak nanocrystalline alignment and magnetic anisotropy. Specifically, we monitor the dynamic magnetic states via real-time magneto-optical Kerr effect measurements across the relevant dynamic phase space as a function of  $H_0$  and  $H_b$ . We find that the qualitative features of the dynamic phase diagram closely follow those of uniaxial Ising-type films. However, the metamagnetic anomalies of the paramagnetic dynamic state, ubiquitous in Ising-type films, appear to be significantly weaker in our nearly isotropic films. Accordingly, the presence of metamagnetic anomalies must be intimately connected with the bistable behavior of Ising systems, which we corroborated by means of detailed analyses of the time-evolution of  $Q$  in the dynamic paramagnetic regime. Thus, the modification of the magnetization state energy landscape that is being facilitated by the nanocrystalline alignment of magnetic grains is crucially important for its dynamic state behavior. In addition, we also investigated the film thickness dependence of the presence or absence of metamagnetic anomalies.

---

**KEYWORDS:** Magnetization reversal, Dynamic phase transitions, Thin films, Nanocrystal order, Magneto-optics

---

**ACKNOWLEDGEMENTS:** This work was supported by the Spanish Ministry of Science and Innovation under the Maria de Maeztu Units of Excellence Program (Grant No. CEX2020-001038-M) and Project No. PID2024-155776NB-I00 (ULTRAMAN).

---

### REFERENCES

- [1] A. Berger, O. Idigoras and P. Vavassori, "Transient Behavior of the Dynamically Ordered Phase in Uniaxial Cobalt Films", *Phys. Rev. Lett.* 111, 190602 (2013).
- [2] M. Quintana and A. Berger, "Experimental Observation of Critical Scaling in Magnetic Dynamic Phase Transitions", *Phys. Rev. Lett.* 131, 116701 (2023).
- [3] P. Riego, P. Vavassori and A. Berger, "Metamagnetic Anomalies near Dynamic Phase Transitions", *Phys. Rev. Lett.* 118, 117202 (2017).
- [4] P. Riego, P. Vavassori and A. Berger, "Towards an understanding of dynamic phase transitions", *Phys. B Condens. Matter* 549, 13 (2018).

## Nanoscale imaging of spin textures with varying altermagnetic response

S. Wintz<sup>1</sup>\*

<sup>1</sup>) Helmholtz-Zentrum Berlin, Germany

\* sebastian.wintz AT helmholtz-berlin.de

Altermagnetism is a recently identified magnetic state in which time-reversal symmetry is broken despite a collinear, fully compensated spin structure [1,2]. The resulting response is governed not only by the d-, g-, or i-wave character of the non-relativistic spin order, but also by the orientation of the Néel vector  $L$ . Spin-orbit-coupling-driven phenomena such as the anomalous Hall effect [3] and X-ray magnetic circular dichroism (XMCD) [4,5] can thus be switched on and off through reorientation of  $L$ , establishing a powerful handle for tuning emergent altermagnetic functionalities. Yet, accessing such  $L$ -dependent responses at the nanoscale has remained experimentally elusive. Here [6], we employ nano-spectroscopic XMCD combined with X-ray magnetic linear dichroism (XMLD) to investigate spin textures with locally varying altermagnetic responses in  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> (hematite), an earth-abundant g-wave altermagnetic candidate [5,7]. By performing spectroscopy across the temperature-driven Morin transition [8], which reorients  $L$  between in-plane and out-of-plane configurations, we observe the switching on-and-off of the XMCD signal, in excellent agreement with DFT+DMFT calculations. While the bulk XMCD vanishes below the Morin temperature, polarization-independent X-ray absorption contrast confirms the Néel vector reorientation and resolves the underlying antiferromagnetic domain configuration. Crucially, nanoscale imaging uncovers a finite XMCD signal at 180° domain walls below the Morin transition, arising from the locally modulated in-plane component of  $L$  within walls otherwise embedded in domains of zero altermagnetic response. Conversely, at room temperature we identify topological meron spin textures [9,10] whose planar regions exhibit XMCD while their nanoscopic, out-of-plane cores show vanishing contrast. These observations demonstrate that nanoscale spin textures can host altermagnetic responses that are qualitatively distinct from those of the surrounding domains. Our results establish  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> as a platform for engineering locally varying altermagnetic functionalities in a light-element, insulating oxide, and open a route toward exploiting complex spin textures-including domain walls and merons-as nanoscale building blocks for altermagnetic spintronics and information processing [11].

**KEYWORDS:** Altermagnetism, X-ray microscopy, Spin textures

### REFERENCES

- [1] L. Šmejkal, J. Sinova, T. Jungwirth, Beyond Conventional Ferromagnetism and Antiferromagnetism: A Phase with Nonrelativistic Spin and Crystal Rotation Symmetry, *Phys. Rev. X* 12, 031042 (2022).
- [2] L. Šmejkal, J. Sinova, T. Jungwirth, Emerging Research Landscape of Altermagnetism, *Phys. Rev. X* 12, 040501 (2022).
- [3] Z. Feng *et al.*, An anomalous Hall effect in altermagnetic ruthenium dioxide, *Nat. Electron.* 5, 735 (2022).
- [4] A. Hariki *et al.*, X-Ray Magnetic Circular Dichroism in Altermagnetic  $\alpha$ -MnTe, *Phys. Rev. Lett.* 132, 176701 (2024).
- [5] E. Galindez-Ruales *et al.*, Revealing the Altermagnetism in Hematite via XMCD Imaging and Anomalous Hall Electrical Transport, *Adv. Mater.* e05019 (2025).
- [6] R. Yamamoto *et al.*, arXiv:2603.09934 (2026).
- [7] O. J. Amin *et al.*, Nanoscale imaging and control of altermagnetism in MnTe, *Nature* 636, 348 (2024).
- [8] F. J. Morin, Magnetic Susceptibility of  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> and  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> with Added Titanium, *Phys. Rev.* 78, 819 (1950).
- [9] F. P. Chmiel *et al.*, Observation of magnetic vortex pairs at room temperature in a planar  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>/Co heterostructure, *Nat. Mater.* 17, 581 (2018).
- [10] H. Jani *et al.*, Antiferromagnetic half-skyrmions and bimerons at room temperature, *Nature* 590, 74 (2021).
- [11] Z. Zhou *et al.*, Manipulation of the altermagnetic order in CrSb via crystal symmetry, *Nature* 638, 645 (2025).

## Printing permanent magnets via room temperature laser transfer

M. Nakano<sup>1</sup>\*

*1) Graduate School of Integrated Science and Technology, Nagasaki University, Japan*

\* mnakano AT nagasaki-u.ac.jp

An annealing process, such as substrate heating and/or post-annealing, is crucial for attaining diverse magnetic properties through crystallization, stress management, anisotropy control, and order transformations. For example, Nd-Fe-B micromagnets produced via sputtering [1] with substrate heating and/or post-annealing have been employed in small devices, and pulsed laser deposition (PLD)-fabricated Nd-Fe-B micro magnets followed by annealing [2] have been developed to minimize the size of electronic devices, including microelectro mechanical systems (MEMS) applications. In this study, micromagnets were prepared without utilizing an annealing process. The reduction in process temperature suggests that micromagnets can be broadly applied, as they can be deposited on flexible materials with low softening points for device applications. Consequently, we conducted fundamental experiments using the laser-induced forward transfer (LIFT) technique, which facilitates 3D printing. The LIFT is a printing technique that employs a pulsed laser beam as the driving force to transfer material from a donor film to a receiving substrate. It has been reported that LIFT can be performed in air and/or at room temperature. Since several researchers reported LIFT-fabricated Cu and Ag films, it has been actively studied due to its high potential for application in fine-electronic devices. The preparation of metals, oxides, and semiconductors has been demonstrated using nanosecond lasers, such as Nd:YAG lasers and excimer lasers. However, as far as we know, there has been limited investigation into LIFT-fabricated permanent magnets. Recently, we reported LIFT-fabricated Nd-Fe-B films in a high vacuum atmosphere and confirmed the transfer of the Nd<sub>2</sub>Fe<sub>14</sub>B crystalline phase from a donor film to the obtained samples on several substrates [3]. This contribution mainly reports the magnetic properties and microstructure of LIFT-made Nd-Fe-B micromagnets.

---

**KEYWORDS:** LIFT technique, Nd-Fe-B micromagnets, Low temperature process

---

**ACKNOWLEDGEMENTS:** This work was supported in part by Japan Society for the Promotion of Science KAKENHI, Japan under Grant JP25K22090 and Grant JP25K01143.

---

### REFERENCES

- [1] N.M. Dempsey, A. Walther, F. May, D. Givord, K. Khlopkov, Gutfleisch O (2007), “High performance hard magnetic NdFeB thick films for integration into micro-electro-mechanical systems,” *Appl. Phys. Lett.*, vol. 90, Art. no. 092509, doi: 10.1063/1.2710771.
- [2] M. Nakano, S. Sato, F. Yamashita, T. Honda, J. Yamasaki, K. Ishiyama, M. Itakura, J. Fiedler, T. Yanai, Fukunaga H (2007), “Review of fabrication and characterization of Nd-Fe-B thick films for magnetic machines,” *IEEE Trans. Magn.*, vol. 43, pp. 2672-2676, doi: 10.1109/TMAG.2007.893778.
- [3] M. Nakano, K. Higashi, G. Tahara, I. Fukuda, A. Yamashita, T. Yanai, K. Nagai, T. Shinshi, Fukunaga H (2024a), “Preparation of Nd-Fe-B films via a low-temperature process,” *IEEE Trans. Magn.*, vol. 60, 2100604, doi: 10.1109/TMAG.2024.3401157.

## Ultra-low iron loss in soft magnetic ribbons by controlling magnetic domain structure and magnetization process

S. Okamoto<sup>1</sup>\*

1) Tohoku University, Japan

\* satoshi.okamoto.e1 AT tohoku.ac.jp

Power electronics has been a key technology for high-efficiency energy conversion in renewable energy, electric mobility, robotics, data centers, power grids, and related applications. Soft magnetic passive devices, such as transformers and inductors, have been crucial elements in power electronics and have become increasingly important in recent years. In particular, reducing iron loss in the high-frequency region is a very important issue. Classically, iron loss has been classified into three components of hysteresis loss, classical eddy-current loss, and excess loss. However, recent studies on high-frequency iron loss have revealed new insights different from the conventional understanding of iron loss. Magnetostriction is a well-known degradation factor of soft magnetic property, and it has been understood to affect static iron loss. However, it is clearly revealed that magnetostriction significantly affects high-frequency iron loss [1]. Since the magnetization process changes with increasing frequency, classification based on magnetization processes is more suitable than the classical iron loss classification method [2].

Very recently, we have successfully demonstrated the ultra-low iron loss in the high-frequency region in both powder core [3] and ribbon sample [4]. Especially, the ultra-low iron loss in the high-frequency region in the ribbon sample is attributed to the realization of a narrow stripe magnetic domain structure with several micrometers in width, which promotes the change in magnetization process from magnetic domain wall displacement to magnetization rotation. Afterward, we found that there are different types of fine magnetic domain structures in soft magnetic amorphous and nanocrystalline ribbons, enabling ultra-low iron loss in the high-frequency region. In this talk, we will present these magnetic domain structures and magnetization process controls in amorphous and nanocrystalline ribbons, and these physical mechanisms.

---

**KEYWORDS:** Soft magnetic material, High-frequency iron loss, Magnetic domain, Magnetization process

---

**ACKNOWLEDGEMENTS:** This work was supported by MEXT Programs of INNOPEL (JPJ009777) and DX-Mag (JPMXP1122715503), and NEDO program (JPNP14015).

---

### REFERENCES

- [1] K. Suzuki, *J. Magn. Magn. Mater.* 592, 171677 (2024).
- [2] N. Ono, et. Al., *J. Magn. Magn. Mater.* 603, 172222 (2024).
- [3] M. Kuno *et al.*, *A. Mater.* 294, 121159 (2025).
- [4] R. Gautam *et al.*, *Nat Commun* 16, 8022 (2025).

## Ultralong-living magnons in YIG for quantum magnonics

R. Serha<sup>1</sup> \*

1) Faculty of Physics, University of Vienna, Vienna, Austria

\* rostyslav.serha AT univie.ac.at

Quantum magnonics (QM) investigates magnons - the quanta of spin waves - as information carriers and interconnects in hybrid quantum systems. Yttrium iron garnet (YIG) is the material of choice due to its exceptionally low magnetic damping. Recent experiments have demonstrated single-magnon detection and quantum control in bulk YIG using superconducting qubits [1, 2]. However, these studies rely on standing ferromagnetic-resonance magnons, whose lifetimes are typically limited to several hundred nanoseconds, restricting scalability and spatial separation of quantum elements. Realization of propagating magnons for QM requires YIG films with long lifetimes at millikelvin temperatures (mK). Most high-quality films are grown on paramagnetic gadolinium gallium garnet (GGG) substrates. At mK, GGG increases damping in the YIG layer and severely degrades YIG/GGG performance [3]. A viable solution is provided by the recently developed diamagnetic garnet substrate, yttrium scandium gallium aluminum garnet (YSGAG), which is lattice-matched to YIG while remaining magnetically inert down to mK. YIG films grown on YSGAG by liquid-phase epitaxy preserve low damping from room temperature down to 30 mK and outperform YIG/GGG films, as well as YIG on other diamagnetic substrates [4]. Additionally, progress has been achieved in bulk systems, where ultra-pure YIG crystals exhibit dipolar-exchange magnons with lifetimes exceeding 18  $\mu$ s at mK [5]. These record values, extracted from nonlinear threshold measurements of three-magnon splitting, demonstrate that magnon dissipation can be suppressed far beyond previously assumed limits. Together, these advances enable ultralong-lived magnons in both YIG films and bulk crystals, and support a materials roadmap toward scalable QM circuits integrating propagating magnons with superconducting qubits, photons, and phonons, including access to nonlinear and nonreciprocal magnon dynamics [4-5].

---

**KEYWORDS:** Quantum magnonics, Yttrium iron garnet, Magnon lifetime, Spin waves, Hybrid quantum systems

---

### REFERENCES

- [1] D. Lachance-Quirion, S. P. Wolski, Y. Tabuchi, *et al.*, "Entanglement-based single-shot detection of a single magnon with a superconducting qubit", *Science* 367, 425 (2020).
- [2] D. Xu, X.-K. Gu, H.-K. Li, *et al.*, "Quantum Control of a Single Magnon in a Macroscopic Spin System", *Phys. Rev. Lett.* 130, 193603 (2023).
- [3] R. O. Serha, A. A. Voronov, D. Schmoll, *et al.*, "Low-damping spin-wave transmission in YIG revealed by the nonlinear threshold", *npj Spintronics* 5, 100025 (2025).
- [4] R. O. Serha, C. Dubs, C. Guguschev, *et al.*, "YIG films on diamagnetic YSGAG substrates for quantum magnonics", *Communications Materials* 10.1038/s43246-026-01146-5 (2026).
- [5] R. O. Serha, K. H. McAllister, F. Majcen, *et al.*, "Ultra-long magnon lifetimes in bulk YIG at millikelvin temperatures", *arXiv:2505.22773* (2025).

## Geometry-Engineered configurational anisotropy in curvilinear 3D magnetic films

O. Bezsmertha<sup>1</sup>, S. Bunyaev<sup>2</sup>, O. V. Pylypovskyi<sup>1</sup>, R. Xu<sup>3</sup>, D. Makarov<sup>1</sup>, G. Kakazei<sup>2\*</sup>

1) Helmholtz-Zentrum Dresden-Rossendorf e.V., Germany

2) Institute of Physics for Advanced Materials, Nanotechnology and Photonics, Portugal

3) Helmholtz-Zentrum Dresden-Rossendorf e.V., 01328 Dresden, Germany., Germany

\* gleb.kakazei AT fc.up.pt

Three-dimensional (3D) nanostructures gained significant attention due to their capability to unlock functionalities beyond the scope of conventional planar systems. Transitioning from planar to 3D architectures provides opportunities to tailor physical properties through geometrical complexity and increased degrees of freedom for material engineering [1-3]. Due to geometry-induced effects stemming from the exchange and magnetostatic interactions, curvilinear nanoarchitectures provide a possibility to design chiral and anisotropic responses, across a wide spatial scale from nanometers to micrometers, determined by the strength and spatial distribution of the geometric curvature. Depositing magnetic film onto a large-area square array of pyramid nanotemplates yields a continuous curvilinear layer with periodic valley/tip topography and a spatially modulated demagnetizing field. Broadband ferromagnetic resonance (FMR) measurements reveal that such 3D topology produces a distinctly nonuniform internal-field landscape and a strongly anisotropic dynamic response that is absent in planar samples. Specifically, the curvilinear film exhibits two distinct resonance branches: a lower-frequency quasi-uniform (Kittel-like) mode and a higher-frequency branch originating from regions of locally enhanced internal field created by the periodic curvature. Angular dependence at different in-plane magnetic fields shows a pronounced fourfold periodicity, directly reflecting the square lattice symmetry of the nanopillars and confirming geometry-induced in-plane anisotropy. A similar four-fold anisotropy has been reported in planar magnonic crystals composed of a square lattice of circular dots beneath a continuous ferromagnetic film, where it arises from the directional variations of the internal effective field [4]. In analogy, the anisotropy observed here originates entirely from the periodic geometric modulation of the continuous magnetic sample. The multi-branch character and anisotropy evolve with applied field: at low fields the spectrum is broadened and complex due to multiple local environments, while increasing field progressively aligns magnetization toward a more uniform configuration but preserves geometry-induced mode splitting until near saturation. Micromagnetic simulations reproduce the observed features and identify valley and tip regions as sources of locally different resonance conditions, linking the additional FMR branch to periodic modulation of the effective field. The geometry-driven configurational anisotropy is sensitive to external field and to geometric/thickness parameters, offering a route to reconfigurable, curvature-engineered magnonic devices.

**KEYWORDS:** Nanomagnetism, Magnetic anisotropy, Ferromagnetic resonance

**ACKNOWLEDGEMENTS:** German team acknowledge support from the European Union's Horizon Europe Research and Innovation Programme (Grant Agreement No. 101070066; REGO project) and from the ERC grant 3DmultiFerro (Project No. 101141331). Portuguese team acknowledge support from FCT - Foundation for Science and Technology through the projects LA/P/0095/2020 (LaPMET), UIDB/04968/2025, and from FEDER - European Regional Development Fund through the project 17142|COMPETE2030-FEDER-00854500.

### REFERENCES

- [1] D. Makarov, O. M. Volkov, A. Kakay, O. V. Pylypovskyi, B. Budinska, O. V. Dobrovolskiy, "New Dimension in Magnetism and Superconductivity: 3D and Curvilinear Nanoarchitectures", *Adv. Mater.* 34, 2101758 (2022).
- [2] D. Raftrey, A. Hierro-Rodriguez, A. Fernandez-Pacheco, P. Fischer, "The road to 3-dim nanomagnetism: Steep curves and architected crosswalks", *J. Magn.Magn. Mater.* 563, 169899 (2022).
- [3] P. Gentile, M. Cuoco, O. M. Volkov, Z.-J. Ying, I. J. Vera-Marun, D. Makarov, and C. Ortix, "Electronic materials with nanoscale curved geometries", *Nat. Electron.* 5, 551 (2022).
- [4] G.N. Kakazei, X.M. Liu, J. Ding, V.O. Golub, O.Y. Salyuk, R.V. Verba, S.A. Bunyaev, A.O. Adeyeye, "Large four-fold magnetic anisotropy in two-dimensional modulated Ni80Fe20 films", *Appl. Phys. Lett.* 107, 232402 (2015).

## Nanoscale YIG-based 2D magnonic crystals

K. Levchenko<sup>1</sup> \*

1) Faculty of Physics, University of Vienna, Vienna, Austria

\* khrystyna.levchenko AT univie.ac.at

Two-dimensional (2D) magnonic crystals (MCs) - magnetic media with periodic geometric modulation in two in-plane directions - provide a platform for engineering spin-wave (SW) dynamics beyond one-dimensional geometries. The 2D periodicity introduces multiple Bragg conditions simultaneously, enabling direction-dependent band gaps and SW scattering between propagation directions [1]. One-dimensional MCs in YIG have already demonstrated well-defined band gaps and frequency-selective SW filtering [2,3], motivating the extension to 2D antidot lattices for richer band structure control and multi-directional transport engineering.

Here, 2D MCs are realised in 100 nm-thick liquid-phase-epitaxy-grown yttrium iron garnet (YIG) films via electron-beam lithography and ion-beam etching of antidot lattices with varying hole diameters and inter-antenna spacings. Defect-free and defect-modulated MCs are studied. In defect-free antidot lattices, propagating spin-wave spectroscopy (PSWS) reveals multiple partially overlapping rejection bands, consistent with Bragg scattering from distinct reciprocal lattice vectors of the 2D structure. Complementary micro-focused Brillouin light scattering ( $\mu$ -BLS) provides spatially resolved SW intensity maps and mode profiles within the unit cell.

In defect-modulated lattices (missing row/column/complex shape between the antennas), local modifications of the periodic potential enable SW transport within the band gap. Line defects form waveguides supporting localised gap modes with partially restored transmission. More complex geometries realise functional SW devices: Y-shaped defects act as stub resonators or notch filters; Mach-Zehnder-type layouts are designed to split the SW beam along two paths of controlled length and recombine it at the output port, where path-length difference can achieve frequency-selective constructive or destructive interference, potentially realising a SW analogue of an optical interferometric switch; and S-shaped channels support guided propagation with bend-induced partial reflections and mode profile modifications.

These results demonstrate nanoscale SW transport governed by lattice symmetry and defect engineering, establishing antidot-lattice MCs as a versatile platform for studying more complex phenomena, like non-trivial edge modes in topological 2D magnonic crystals [4].

---

**KEYWORDS:** 2D magnonic crystals (MCs), Yttrium iron garnet (YIG) films, Antidot lattice, Nanoscale, Spin-wave routing

---

**ACKNOWLEDGEMENTS:** This work was supported by the Austrian Science Fund (FWF) [10.55776/ESP526].

---

### REFERENCES

- [1] M. Krawczyk and D. Grundler, *J. Phys.: Condens. Matter* 26 , 123202 (2014).
- [2] K. O. Levchenko *et al.*, *Appl. Phys. Lett.* 127 , 172401 (2025).
- [3] K. O. Levchenko *et al.*, *IEEE Trans. Mag.* DOI: 10.1109/TMAG.2026.3657608 (2026).
- [4] R. Shindou *et al.*, *Phys. Rev. B* 87 , 174427 (2013).

## Microscale spin-wave devices for next-generation 6G radio-frequency signal processing

A. Chumak<sup>1</sup>\*

1) Faculty of Physics, University of Vienna, Vienna, Austria

\* andrii.chumak AT univie.ac.at

Wireless communication continues to push toward higher frequencies and smaller form factors, demanding radio-frequency (RF) components that handle ever-broader spectra without growing in size or power consumption. As 5G and 6G networks expand from sub-6 GHz bands into Frequency Range 2 (FR<sub>2</sub>, 24-71 GHz) and the proposed Frequency Range 3 (FR<sub>3</sub>, 7-24 GHz), conventional electronic and acoustic technologies are reaching fundamental performance ceilings.

Spin waves - collective magnetic excitations in ferromagnets - operate naturally in the GHz-to-THz range, can be miniaturized to the micro- and nanoscale, and offer a single magnonic platform on which filters, delay lines, frequency-selective limiters, and reconfigurable signal-processing functions coexist [1]. Yttrium iron garnet (YIG), whose low magnetic damping ( $\sim 3 \times 10^{-4}$ ) supports spin-wave propagation over hundreds of micrometers to several millimeters, is the material of choice. Yet their deployment has been constrained by significant insertion losses, dominated by inefficient electromagnetic-to-spin-wave conversion at the transducers [2,3].

In this talk I will overview our recent progress on microscale spin-wave RF devices - including a nanoscale frequency-selective limiter [2] and high-frequency delay lines [3] - and then show that the insertion loss of YIG-based U-shaped transducers can be systematically minimized at every operating frequency across 5-30 GHz by tuning the transducer geometry, reaching 6.25 dB at 12 GHz.

The optimum shifts continuously with frequency because the ohmic-inductive transducer impedance and the spin-wave radiation impedance evolve oppositely with frequency. Mapping this matching landscape across more than one hundred device geometries, and benchmarking the data against micromagnetic simulations [4], yields explicit design rules linking any target frequency to a specific transducer geometry. These guidelines - transferable to limiters, filters, and delay lines on the same chip - bring spin-wave RF components close to the performance required for 5G FR<sub>3</sub> signal processing and open a path toward compact, energy-efficient magnonic RF front-ends.

---

**KEYWORDS:** Magnonics, Spin-wave devices, RF applications

---

**ACKNOWLEDGEMENTS:** The research is being conducted as part of the ERC Proof of Concept project 5G-Spin, and with the support of the Austrian promotional bank (AWS), as part of the "Spin-wave RF filters for 5G communication systems" project.

---

### REFERENCES

- [1] Levchenko, Davidková, Mikkelsen, Chumak (2026). Review on spin-wave RF applications. IEEE Transactions on Magnetism.
- [2] Davidková, Levchenko, Bruckner *et al.* (2025). Nanoscale spin-wave frequency-selective limiter for 5G technology. Phys. Rev. Applied 23, 034026.
- [3] Davidková, Levchenko, Serha *et al.* (2025). Spin-wave microscale RF delay lines for mid- and high-frequency 5G band. J. Appl. Phys. 138, 143908.
- [4] Bruckner, Davidková, Abert *et al.* (2025). Micromagnetic simulation and optimization of spin-wave transducers. Sci. Rep. 15, 19993.

## Spatial and temporal coherence of magnon Bose-Einstein condensates

M. R. Schweizer<sup>1</sup> \*

1) *Fachbereich Physik and Landesforschungszentrum OPTIMAS, Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, 67663 Kaiserslautern, Germany*

\* mschweiz AT rptu.de

Magnons are the quanta of spin waves, i.e., delocalized excitations in a lattice of spins. As bosons, they adhere to the Bose-Einstein distribution, which leads to the formation of a condensate at the fundamental energy state whenever the number of (quasi-)particles exceeds the capacity of the gas state. As the condensate's order parameter, the condensate phase is expected to transition to a coherent state in the process of condensation. However, since the first observation of a magnon condensate [1], experimental access to this property has remained elusive.

Since the coherence of a condensate is reflected in a well-defined phase state both in time and space, the challenge of accessing the condensate phase breaks down into two complementary aspects. Temporal coherence becomes apparent through phase-sensitive, time-resolved measurements that reveal the spontaneous emergence of a stable oscillation frequency and a randomly chosen initial phase. Using such a phase-referenced, electrical measurement technique, we provide experimental evidence for strong temporal correlations of the condensate signal and randomized initial phase selection during condensation [2].

In contrast, spatial coherence manifests in the condensate's response to potential landscapes imprinted onto the condensate. Here, spatially modulated magnetization profiles [3] impose phase gradients that drive magnon currents within the condensate. Using Brillouin light scattering spectroscopy with both spatial and temporal resolution, we demonstrate that a redistribution of magnons can be observed within an artificially created magnetization landscape acting as a potential profile [4-5].

Together, these results provide evidence for both temporal and spatial coherence in magnon Bose-Einstein condensates, opening new pathways for controlling phase-driven dynamics in magnonic systems.

---

**KEYWORDS:** Magnonics, Bose-Einstein-Condensation, Phase, Coherence

---

**ACKNOWLEDGEMENTS:** We acknowledge support from the European Research Council (ERC) under the European Union's Horizon Europe research and innovation programme (Grant agreement No. 101044526). This study was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation), TRR 173-268565370 Spin+X (Project B04 and B13), as well as by grant DMR-2338060 from the National Science Foundation of the United States.

---

### REFERENCES

- [1] S. O. Demokritov, V. E. Demidov, O. Dzyapko, G. A. Melkov, A. A. Serga, B. Hillebrands, and A. N. Slavin, “Bose-Einstein condensation of quasi-equilibrium magnons at room temperature under pumping”, *Nature*, 443, 430 (2006).
- [2] M. Koster, M. R. Schweizer, T. Noack, V. I. Vasyuchka, D. A. Bozhko, B. Hillebrands, M. Weiler, A. A. Serga, and G. von Freymann, “Spontaneous Emergence of Phase Coherence in a quasiparticle Bose-Einstein Condensate”, arXiv:2507.16862 (2025).
- [3] M. R. Schweizer, F. Kühn, M. Koster, G. von Freymann, B. Hillebrands, and A. A. Serga, “Rapid-prototyping of microscopic thermal landscapes in Brillouin light scattering spectroscopy”, *Rev. Sci. Instrum.*, 94, 093903, (2023).
- [4] M. R. Schweizer, F. Kühn, V. S. L'vov, A. Pomyalov, G. von Freymann, B. Hillebrands, and A. A. Serga, “Local temperature control of magnon frequency and direction of supercurrents in a magnon Bose-Einstein condensate”, *Appl. Phys. Lett.*, 124, 092402 (2024).
- [5] M. R. Schweizer, A. J. E. Kreil, G. von Freymann, B. Hillebrands, and A. A. Serga, “Confinement of Bose-Einstein magnon condensates in adjustable complex magnetization landscapes”, *J. Appl. Phys.*, 132, 183908 (2022).

## Inter-particle interactions in magnetic hyperthermia: Clustering, agglomeration and calorimetric SAR estimation

S. I. Ruta<sup>1</sup>\*

1) Sheffield Hallam University, United Kingdom

\* sergiu.ruta AT shu.ac.uk

Magnetic hyperthermia is an emerging magnetothermal strategy in which magnetic nanoparticles are delivered to a target region and exposed to an alternating magnetic field, generating local heat. Although developed mainly for cancer treatment, magnetic nanoparticle-mediated heating is increasingly explored for thermally triggered drug release, magnetogenetic control of cellular activity, and cryopreserved tissue/organ rewarming. Heating efficiency is commonly quantified by the specific absorption rate (SAR) or specific loss power (SLP). However, SAR/SLP depends not only on particle size, anisotropy and magnetisation, but also on inter-particle interactions, clustering, agglomeration and field-induced reorganisation.

In this talk, I will focus on three connected aspects: experimental evidence of nanoparticle agglomeration in cellular environments, simulations of clustering-dependent SLP, and theoretical-experimental approaches for improved SLP estimation.

Recent experiments have shown that magnetic nanoparticles do not always remain uniformly dispersed under alternating magnetic fields [1]. Vesicles containing magnetic nanoparticles, appear relatively evenly distributed before field exposure, but reorganise into field-aligned chains when the field is applied. Once the field is removed, this organisation relaxes, indicating dynamic and reversible clustering. This suggests that particle arrangement can evolve during hyperthermia. We simulated nanoparticle clustering and examined how prescribed aggregate morphologies influence heating[1]. Our results show that chain formation and local concentration strongly affect SAR/SLP [2], highlighting the importance of inter-particle interactions.

This requires robust SLP estimation and, where possible, the ability to monitor time-dependent changes in SLP during field exposure. Our work has shown that conventional Newton-law-based approaches can introduce large uncertainty when temperature gradients and multiple heat-loss pathways are present. To address this, the Peak Analysis Method [3] estimates SLP from the field on/off temperature peak using a heat-diffusion framework, making it suitable when Newton's law of cooling is invalid. The protocol was validated using heat-diffusion simulations of the liquid sample, holder and surrounding air, and tested experimentally on three devices in different laboratories, improving SLP determination compared with initial-slope, Box-Lucas and Corrected Slope methods. Implemented in a zigzag heating-cooling protocol, it enables repeated SLP estimation and monitoring of heating changes over time or temperature. More recently, the method has been extended into freely accessible online software [4], combining Peak Analysis with statistically guided fitting to reduce subjectivity and support wider use.

---

**KEYWORDS:** Magnetic nanoparticles, Magnetic hyperthermia, SLP, SAR, Agglomeration

---

### REFERENCES

- [1] Fernández-Afonso, Yilian, Sergiu Ruta, Amira Pérez-Rodríguez, Thomas S. van Zanten, Sian Gleadhall, Raluca M. Fratila, María Moros *et al.* "Reversible alignment of nanoparticles and intracellular vesicles during magnetic hyperthermia experiments." *Advanced Functional Materials* 34, no. 40 (2024): 2405334.
- [2] Ruta, Sergiu, R. Chantrell, and O. Hovorka. "Unified model of hyperthermia via hysteresis heating in systems of interacting magnetic nanoparticles." *Scientific reports* 5, no. 1 (2015): 9090.
- [3] Ruta, Sergiu, Yilian Fernández-Afonso, Samuel E. Rannala, M. Puerto Morales, Sabino Veintemillas-Verdaguer, Carlton Jones, Lucía Gutiérrez, Roy W. Chantrell, and David Serantes. "Beyond Newton's law of cooling in evaluating magnetic hyperthermia performance: a device-independent procedure." *Nanoscale Advances* 6, no. 16 (2024): 4207-4218.
- [4] López-Vázquez, Iago, Yilian Fernández-Afonso, Antonio Santana-Otero, Sergiu Ruta, Alfredo Amigo, M. Puerto Morales, Roy W. Chantrell, Lucía Gutiérrez, and David Serantes. "SLPcalculator: a web-based tool to estimate nanoparticle heating with peak analysis and F-test." *Nanoscale* 18, no. 9 (2026): 4790-4799.

## Magnetic tunnel junction assemblies for logic devices

S. Majetich<sup>1</sup>\*, C. Sullivan<sup>1</sup>

1) Carnegie Mellon University, USA

\* sara AT cmu.edu

Artificial spin ice (ASI) has potential for application as low power logic and computing devices, and there have been numerous demonstrations using external magnetic fields. When the magnetostatically coupled nanomagnets are the free layers of magnetic tunnel junctions (MTJs), there are multiple options for electrical control of inputs, including spin torque and voltage-control of magnetic anisotropy as well as a simple Oersted field, and magnetoresistance can be used to detect the outputs. However, it is challenging to control the propagation of injected excitations without an external magnetic field. Here we describe the design of MTJ ASI in order to promote field-free propagation.

Square lattice ASI made from 60 nm circular MTJs shows field-free fluctuations at  $H = 0$  [1]. Here there is no shape anisotropy and symmetry is broken by a small coupling field from the fixed layer. Tunnel magnetoresistance (TMR) is able to distinguish eleven different magnetization angles of the free layer moments, which are explained by a model of near and next nearest neighbor magnetostatic interactions. While high energy “emergent magnetic monopole” configurations are frequently detected, there is only a small driving force for propagation across the array, which comes from the coupling field.

Two promote propagation, a small amount of shape anisotropy in the MTJ free layers is introduced and the angle between their easy axes and the magnetization of the pinned fixed layer is varied. An elliptical nanomagnet with an easy axis at an angle relative to the applied field reverses through a combination of rotation and switching, as seen in micromagnetic simulations. However, when the fixed layer moment is along the field direction, the switching of the free layer is nearly symmetric, leading to nearly zero change in TMR. For measurable changes in TMR while switching the coupling field must be at an angle to the applied field. An additional benefit of changing the angle of the coupling field is the reduction of the energy barrier, which was found to be a minimum at  $45^\circ$  for 60 nm x 90 nm half-patterned MTJs [2]. For external field-free propagation, only the magnetostatic field from the near neighbors plus the coupling field of the fixed layer can be used to propagate injected excitations. Micromagnetic simulations are used to predict the magnetostatic fields due to near neighbors and compared with the angle-dependent coercivities to design optimal ASI. Propagation is tested using hard-wired inputs switched by spin transfer torque to inject excitations, which are detected at different locations in the ASI using TMR measured by conductive atomic force microscopy.

---

**KEYWORDS:** Magnetic tunnel junctions, Artificial spin ice, Spintronic logic, Magnetoresistance, Spin-torque

---

### REFERENCES

- [1] C. Sullivan, H. Chen, Y. Wen, Q. Zhang, X. X. Zhang, and S. A. Majetich, Phys. Rev. Appl. 25, 044049 (2026).
- [2] H. Chen, B. Parks, Q. Zhang, B. Fang, X. X. Zhang, and S. A. Majetich, Appl. Phys. Lett. 120, 212401 (2022).

## Magnetism in metastable actinide compounds: Thin films as a gateway to inaccessible ground states

E. Tereshina-Chitrova<sup>1\*</sup>, S. G. Alex<sup>1</sup>, O. Koloskova<sup>1</sup>, L. Horak<sup>2</sup>, L. Havela<sup>2</sup>, F. Huber<sup>3</sup>, T. Gouder<sup>3</sup>

1) Institute of Physics of the Czech Academy of Sciences, Czech Republic

2) Charles University, Faculty of Mathematics and Physics, Czech Republic

3) European Commission, Joint Research Centre (JRC) Karlsruhe, Germany

\* teresh AT fzu.cz

Actinide materials host some of the most complex magnetic phenomena in condensed matter physics, arising from the competition between relativistic, correlation, and hybridization effects on the  $5f$  states. In uranium compounds, multiple electronic and magnetic configurations frequently lie close in energy, rendering the ground state highly sensitive to structural perturbations and chemical environment. Thin-film growth offers a fundamentally distinct regime from bulk synthesis by enabling non-equilibrium stabilization [1,2], interface coupling, and controlled strain engineering [3] - effects that can drive uranium systems toward magnetic and electronic states inaccessible in equilibrium bulk compounds. We demonstrate this behavior in uranium hydrides [1] and chalcogenides [4] prepared by reactive sputtering. A representative example is metastable  $\text{UH}_2$ , stabilized exclusively in thin-film form [1], in which magnetometry and element-specific spectroscopy reveal robust ferromagnetism accompanied by strong orbital contributions to the uranium  $5f$  moment. These findings establish thin-film actinide materials as an independent experimental platform for exploring hidden crystallographic and magnetic phases and emergent  $5f$  ground states beyond the reach of conventional bulk thermodynamics.

---

**KEYWORDS:** Thin films synthesis, Uranium compounds, Magnetism, Metastable states

---

**ACKNOWLEDGEMENTS:** We acknowledge the support of Czech Science Foundation under the grant No. 26-20860S. The samples were prepared in the framework of the EARL project of the European Commission Joint Research Centre, ITU Karlsruhe. Physical properties measurements were performed in the Materials Growth and Measurement Laboratory (<http://mgml.eu>) supported within the program of Czech Research Infrastructures (Project No. LM2023065).

---

### REFERENCES

- [1] A. Evgenia. Tereshina-Chitrova *et al.*, Spin and orbital magnetism in  $\text{UH}_2$  thin films studied by X-ray magnetic circular dichroism, *Applied Surface Science* 736 (2026) 166753.
- [2] S.G. Alex *et al.*, Electronic structure of  $\text{UGe}_{2\pm x}$  thin films from photoelectron spectroscopy, *J. Electron Spectrosc. Relat. Phenom.*, 286 (2026) 147611.
- [3] E. A. Tereshina-Chitrova *et al.*, Strain-driven Switching Between Antiferromagnetic States in Frustrated Antiferromagnet  $\text{UO}_2$  Probed by Exchange Bias Effect, *Adv. Funct. Mater.* 34 (2024) 2311895.
- [4] E.A. Tereshina-Chitrova *et al.*, Photoelectron spectroscopy study of U-Te thin films: A unified perspective of hybridization effects across compositions, *Materials Today Communications* 53 (2026) 115238.

## Magnetic properties and detection of the electronic states for half-metallic ferromagnets in Heusler alloys

R. Y. Umetsu<sup>1</sup>\*

*1) Institute for Materials Research, Tohoku University, Japan*

\* rie.umetsu AT tohoku.ac.jp

Since half-metallic electronic structures were theoretically predicted in some half-Heusler and full-Heusler alloys [1,2], the half-metallic ferromagnets have been intensively investigated in a field of spintronics. Soft X-ray resonant inelastic X-ray scattering (RIXS) and the magnetic circular dichroism (MCD) were performed in order to detect the half-metallic electronic states in Heusler alloys [3-5]. Because the RIXS is a photon-in/ photon-out spectroscopy technique using a high-brilliance synchrotron light source, it allows us to probe the electronic structures in an elemental specific way by tuning the incoming photon energy.

The RIXS-MCD measurements were performed at SPring-8 BL<sub>07</sub>LSU and NanoTerasu BL<sub>07</sub>U using left and right circularly polarized light. It has been clarified important information related to the electronic states around the Fermi level can be obtained by systematic studies in some Heusler alloys.

Single crystals of some Heusler alloys were grown by the Bridgeman method. The crystal orientation was checked using Laue's back reflection method and the specimen was cut into stripes in the direction parallel to the  $\langle 100 \rangle$ .

It was found that the Zeeman energy, width of the gap formed at the Fermi level, and which spin band opens the half-metallic gap can be revealed from comparison between experimental and theoretical spectra of RIXS-MCD. Furthermore, the RIXS-MCD experiments at the new synchrotron facility in Japan, NanoTerasu, were performed for Co<sub>2</sub>MnGa alloy, which has been known as a Weyl ferromagnet. Because of the brilliant light at NanoTerasu and the higher resolution of spectra, clearer structures could be observed especially in Co-*L* edge. Interestingly, it was found that the Mn-3*d* orbitals behave half-metallic character around the Fermi level, on the contrary, the Co-3*d* ones exhibit metallic band character at both spin states. These findings suggest that the Weyl crossing would be caused by the Co-3*d* electrons.

---

**KEYWORDS:** Half-metallic ferromagnet, Heusler alloy, RIXS-MCD, NanoTerasu

---

**ACKNOWLEDGEMENTS:** The author sincerely thanks T. Sugawara and Y. Murakami in IMR, Tohoku Univ. for their help to make single crystals and composition analyses, and Emeritus Prof. T. Kanomata in Tohoku-Gakuin Univ. for valuable discussions. The RIXS-MCD experiments were performed under cooperative research works with groups of the Univ. Osaka (H. Fujiwara, S. Suga, and T. Oguchi), AIST (F. Kuroda), the Univ. Tokyo (H. Kiuchi, W. Zhang, and S. Harada) and QST (J. Miyawaki).

---

### REFERENCES

- [1] R.A. de Groot, F. M. Mueller, P. G. van Engen, and K. H. J. Buschow, “New Class of Materials: Half-Metallic Ferromagnets”, *Phys. Rev. Lett.* 50, 2024 (1983)
- [2] S. Ishida, S. Akazawa, Y. Kubo, and J. Ishida, “Band theory of Co<sub>2</sub>MnSn, Co<sub>2</sub>TiSn and Co<sub>2</sub>TiAl” *J. Phys. F* 12, 1111 (1982)
- [3] K. Nagai, H. Fujiwara, H. Aratani, S. Fujioka, H. Yomosa, Y. Nakatani, T. Kiss, A. Sekiyama, F. Kuroda, H. Fujii, T. Oguchi, A. Tanaka, J. Miyawaki, Y. Harada, Y. Takeda, Y. Saitoh, S. Suga, and R. Y. Umetsu, “Electronic structure and magnetic properties of the half-metallic ferrimagnet Mn<sub>2</sub>VAI probed by soft x-ray spectroscopies”, *Phys. Rev. B* 97, 035143 (2018).
- [4] R. Y. Umetsu, H. Fujiwara, K. Nagai, Y. Nakatani, M. Kawada, A. Sekiyama, F. Kuroda, H. Fujii, T. Oguchi, Y. Harada, J. Miyawaki, and S. Suga, “Half-metallicity of the ferrimagnet Mn<sub>2</sub>VAI revealed by resonant inelastic soft x-ray scattering in a magnetic field”, *Phys. Rev. B* 99, 134414 (2019).
- [5] H. Fujiwara, R. Y. Umetsu, F. Kuroda, J. Miyawaki, T. Kashiuchi, K. Nishimoto, K. Nagai, A. Sekiyama, A. Irizawa, Y. Takeda, Y. Saitoh, T. Oguchi, Y. Harada, S. Suga, “Detecting halfmetallic electronic structures of spintronic materials in a magnetic field”, *Sci. Rep.* 11, 18654 (2021).

## GPU-accelerated inverse micromagnetics: From billion-cell simulations to magnonic device optimization

D. Suess<sup>1</sup>\*

*1) Faculty of Physics, University of Vienna, Austria*

\* dieter.suess AT univie.ac.at

We present a unified GPU-accelerated framework for inverse micromagnetics, built on auto-differentiable solvers in JAX and PyTorch, and demonstrate its application across three distinct inverse-design challenges: magnetization reconstruction from stray-field data, topology optimization of magnonic devices, and loss optimization in spin-wave transducer systems.

The computational foundation is provided by our micromagnetic solvers magnum.np [1], and NeuralMag [2], jaxFD (finite-difference) and jaxFE (finite-element, based on the Fast Multipole Method) [3]. On 8 NVIDIA B<sub>200</sub>-192GB GPUs, we demonstrate stray-field evaluation of a 15043 cube (3.4 billion cells) in 492 ms, and transient dynamics of a billion-cell Permalloy cube at roughly one minute of computation per nanosecond of physical time.

Building on these differentiable solvers, we show that micromagnetic energy can serve as a physics-informed regularizer for inverse magnetostatic problems. Applied to nitrogen-vacancy magnetometry data of Fe<sub>3</sub>-xGaTe<sub>2</sub>, our framework jointly reconstructs the magnetization texture and the unknown sensor-sample distance through gradient-based optimization on the unit-sphere manifold [4].

For dynamic inverse-design problems, we combine a level-set parameterization with the adjoint-state method to perform topology optimization of magnonic devices with constant memory footprint. This is demonstrated by the design of a 300 nm-wide YIG demultiplexer achieving frequency-selective spin-wave separation [5].

Finally, applying the inverse framework to spin-wave transducer systems, we decompose the total insertion loss into reflection, ohmic, propagation, and directional contributions. This systematic loss separation, validated against experimental S-parameter data from YIG-based devices, identifies ohmic losses as the dominant mechanism and guides transducer geometry optimization. Together, these results establish GPU-accelerated inverse micromagnetics as a versatile toolchain bridging static reconstruction, dynamic optimization, and device engineering at scales previously inaccessible to micromagnetic simulation.

---

**KEYWORDS:** Inverse micromagnetics, Magnonics, GPU-accelerated simulation, Topology optimization, Spin waves

---

### REFERENCES

- [1] F. Bruckner *et al.*, Sci. Rep. 13, 12054 (2023).
- [2] C. Abert *et al.*, npj Comput. Mater. (2025).
- [3] R. Kraft *et al.*, arXiv:2511.15269 (2025).
- [4] A. Setescak *et al.*, submitted.
- [5] A.A. Voronov *et al.*, npj Spintronics 3, 19 (2025).

## Electric excitation of magnetic resonance in altermagnets

R. Ramazashvili<sup>1</sup>, V. Shablenko<sup>2</sup>, Y. Bazaliy<sup>2\*</sup>

1) *Universite Paul Sabatier, France*

2) *University of South Carolina, USA*

\* bazaliy AT mailbox.sc.edu

Magnetic resonance is conventionally excited by the radio-frequency oscillating magnetic fields. Electric fields do not couple to the magnetic moment and have no direct influence on it. However, in altermagnets the exchange splitting depends on electron's momentum, and thus electron's acceleration, induced by the electric field, leads to the emergence of an effective magnetic field acting on the spin. In this talk we will present a simple model of an altermagnet where such electrically induced spin resonance is possible and discuss the prospects of its observation.

---

**KEYWORDS:** Altermagnets, Spin resonance, Electric-field control, Spintronics

## Spin-polarised surface plasmon polaritons generated at an oxide/metal interface

A. Y. Lee<sup>1</sup>, H. Koizumi<sup>2</sup>, E. Moedl<sup>3</sup>, D. Oue<sup>4</sup>, M. Matsuo<sup>5</sup>, A. Hirohata<sup>1, 6 \*</sup>

1) Tohoku University, Japan

2) University of Tsukuba, Japan

3) RWTH Aachen University, Germany

4) RIKEN, Japan

5) Kavli Institute for Theoretical Sciences, China

6) Max Planck Institute, Germany

\* atsufumi.hirohata.d1 AT tohoku.ac.jp

Surface plasmon polaritons (SPPs) have attracted significant attention as a platform for coupling spintronic and opto-spintronic devices [1]. SPPs enable a strong interaction at a metal/insulator interface and allow electromagnetic fields to be confined beyond the diffraction limit. SPPs are generated in a PHz regime in a non-magnetic metal, which can generate a magnetisation gradient and a resulting spin current. In this study, SPP-induced spin currents were measured via the inverse spin Hall effect (ISHE). A thin Ag-layer was deposited on a oxide substrate, including SiO<sub>2</sub>, Y-Fe<sub>2</sub>O<sub>3</sub> and MgO, using ultra-high vacuum sputtering. Here Ag exhibited the largest SPP signals among the investigated series of metals. By placing a half-cylindrical prism at the center of the sample, a laser beam was introduced at an elevating incident angle between 20 and 70 degrees from the film plane. The laser incidence was linearly-polarised to generate both *s*- and *p*-polarisations. The spot size of the incident beam was then controlled using an objective lens. For the inverse spin Hall measurement, a source meter (Keithley, 2400) was used to detect the spin Hall voltage by connecting electrical contacts at the diagonal corners of the continuous films. The measurements were carried out with up to 150 repetitions with 2 s interval to eliminate the Joule heating by laser introduction at each angle. For a Ag/SiO<sub>2</sub> sample, we detected a clear Hall voltage signal showing a pronounced dependence on the incident angle. A well defined maximum was measured to appear at approximately 52 degrees, which agrees with the theoretical prediction [1].

---

**KEYWORDS:** Surface plasmon polaritons, Inverse spin Hall effect, Oxides

---

**ACKNOWLEDGEMENTS:** This work was supported by the Cooperative Research Project from the Center for Science and Innovation in Spintronics (Core Research Cluster) of Tohoku University, the Japan Science and Technology Agency (JST) Adopting Sustainable Partnerships for Innovative Research Ecosystem (ASPIRE) programme (No. JPMJAP2409) and the Ministry of Education, Culture, Sports, Science and Technology (MEXT) X-nics (Grant No. JPJ011438).

---

### REFERENCES

[1] D. Oue and M. Matsuo, J. New. Phys. 22, 033040 (2020).

## Evolution of Mn-derived states in alloyed (III,Mn)V semiconductors

O. Yastrubchak<sup>1\*</sup>, N. Tataryn<sup>1</sup>, S. Mamykin<sup>1</sup>, Y. Ichiyanagi<sup>2</sup>, O. Fedchenko<sup>3</sup>, O. Tkach<sup>4</sup>, Y. Lytvynenko<sup>4</sup>, V. Romanyuk<sup>1</sup>, L. Borkovska<sup>5</sup>, O. Kondratenko<sup>1</sup>, L. Khomenkova<sup>1</sup>, X. Liu<sup>6</sup>, T. Wosinski<sup>7</sup>, J. Furdyna<sup>6</sup>, J. Sadowski<sup>8</sup>, G. Schönhense<sup>4</sup>, B. A. Assaf<sup>6</sup>, H. Elmers<sup>4</sup>

1) V.E. Lashkaryov Institute of Semiconductor Physics, National Academy of Sciences of Ukraine, pr. Nauky 41, 03028, Kyiv, Ukraine, Ukraine

2) Department of Physics, Graduate School of Engineering Science, Yokohama National University, Yokohama, Kanagawa 240-8501, Japan, Japan

3) Physikalisches Institut, Goethe Universität Frankfurt, Germany

4) Johannes Gutenberg-Universität Mainz, Institut Für Physik, 55128 Mainz, Germany, Germany

5) V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine, Ukraine

6) Department of Physics and Astronomy, University of Notre Dame, Notre Dame, IN 46556 USA, USA

7) Institute of Physics Polish Academy of Sciences, Poland

8) Institute of Physics, Polish Academy of Sciences, Poland

\* plazmonoki AT gmail.com

Ferromagnetic semiconductors (FMSs) based on (III,Mn)V alloys have long served as model systems for exploring spin-charge interactions and engineered magnetic functionalities. In ternary III-Mn-V alloys, Mn provides both the magnetic moments and the charge carriers that enable itinerant hole-mediated magnetic order. As a result, modifying the electronic structure without simultaneously changing the concentration of magnetic species remains challenging.

Alloying the (Ga,Mn)As matrix with elements such as In, P, or Bi provides an additional route for engineering the electronic structure through modifications of lattice parameters and band alignment [1-4]. A central issue in (III,Mn)V systems concerns the nature of the Mn-derived electronic states. In particular, it remains unclear whether Mn forms weakly coupled impurity-like states or states that are strongly hybridized with the host valence band. The degree of hybridization between Mn 3d states and anion p states of the host lattice governs this behavior. In turn, it determines both the character of the Mn-derived states and the mechanism of exchange interactions, ranging from impurity-like exchange in the weak-hybridization limit to valence-band-mediated interactions in the strong-hybridization regime.

In the present study, we combine spectroscopic ellipsometry (SE) and hard X-ray angle-resolved photoemission spectroscopy (HARPES) to investigate the impact of In, Bi, and P incorporation, as well as post-growth annealing, on the electronic structure of (In,Ga,Mn)As, (Ga,Mn)(As,Bi), and (Ga,Mn)(As,P), respectively.

The combined optical and photoemission results provide a coherent picture of how phosphorus incorporation modifies the character of Mn levels in (Ga,Mn)(As,P). The nature of the Mn-induced acceptor state evolves as a function of its energetic separation from the valence-band maximum. The evolution of this energy separation with increasing P concentration can be directly visualized using HARPES. When the acceptor level lies close to the valence-band edge, the Mn states retain a predominantly hybridized, valence-band-like character and remain partially delocalized over neighboring anion sites. As the valence-band edge shifts further away from the Mn levels with increasing P content, the Mn states become progressively more Mn-centered. This results in stronger localization on the Mn 3d orbitals and ultimately leads to the formation of a distinct impurity band.

**KEYWORDS:** Ferromagnetic semiconductors, P-d hybridization, P) alloys, Hard X-ray angle-resolved photoemission spectroscopy (HARPES), Spectroscopic ellipsometry (SE)

**ACKNOWLEDGEMENTS:** BAA and XL acknowledge support from National Science Foundation grant DMR-2313441. O.Y., N.T., O.K., V.R., L.B., L.Kh. and S.M. acknowledge the National Research Foundation of Ukraine for financial support of this research (Project number 2025.07/0271). OY is partly supported by a Fulbright Fellowship through the US Department of State. Funding by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation), grant no. TRR 173 268565370 (project A02) is gratefully acknowledged, as well as the funding of the instrument by the Federal Ministry of Education and Research (BMFTR) under the framework program ErUM (projects 05K25UM1 and 05K25UMA). We thank DESY (Hamburg, Germany), a member of the Helmholtz Association HGF, for the provision of experimental facilities. Parts of this research were performed at PETRA III using beamline P22. YI acknowledges support from Japan Science and Technology Agency (JST) - Mirai Program under Grant JPMJMI17D7, the Grant-in-Aid for Scientific Research from Japan Society for the Promotion of Science (JSPS) under Grant Kiban(A) 20H00344, and Japan Agency for Medical Research Development (AMED) H48.

## REFERENCES

- [1] L. Sawicki, D. Gluba, S. Vasilyev, S. Babenkov, A. Chernov, H.J. Winkelmann, G. Elmers, Schönhense, “Site-specific atomic order and band structure tailoring in the diluted magnetic semiconductor (In,Ga,Mn)As,” *Phys. Rev. B*, 103, 075107 (2021).
- [2] N. Tataryn, L. Gluba, O. Yastrubchak, J. Sadowski, T. Andrearczyk, S. Mamykin, M. Sawicki, T. Wosinski, “Valence Band Dispersion in Bi-Doped (Ga,Mn)As Epitaxial Layers,” *IEEE Trans. Magn.*, 59, 4100405 (2023).
- [3] O. Yastrubchak, N. Tataryn, L. Gluba, S. Mamykin, J. Sadowski, T. Andrearczyk, J. Z. Domagala, O. Kondratenko, V. Romanyuk, O. Fedchenko, Y. Lytvynenko, O. Tkach, D. Vasilyev, S. Babenkov, K. Medjanik, K. Gas, M. Sawicki, T. Wosinski, G. Schönhense, H.-J. Elmers, “Influence of Bi doping on the electronic structure of (Ga,Mn)As epitaxial layers,” *Sci. Rep.*, 13, 17278 (2023).
- [4] O. Yastrubchak, L. Riney, W. Powers, N. Tataryn, S. Mamykin, O. Kondratenko, V. Romanyuk, L. Borkovska, O. Kolomys, L. Khomenkova, J. Wang, X. Liu, J.K. Furdyna B.A. Assaf, “Band Engineering of Magnetic (Ga,Mn)As Semiconductors by Phosphorus Doping,” *IEEE Trans. Magn.*, 59, 1600106 (2023).

## Structure formation and magnetic properties of Gd-doped yttrium iron ferrites

Y. Shlapa<sup>1\*</sup>, O. Tovstolytkin<sup>2</sup>, M. Popov<sup>3</sup>, A. Belous<sup>1</sup>

1) V. Vernadsky Institute of General and Inorganic Chemistry, NAS of Ukraine, Ukraine

2) V.G. Baryakhtar Institute of Magnetism of the NAS of Ukraine, Ukraine

3) Educational and Scientific Institute of High Technologies, Taras Shevchenko National University of Kyiv, Ukraine

\* yuliashlapa AT ukr.net

Ultra-high frequency (UHF) ferrites are essential materials for modern communication and radiolocation systems, particularly in emerging technologies such as 5G networks, where high signal stability, low losses, and miniaturization are required. Yttrium iron garnet ( $\text{Y}_3\text{Fe}_5\text{O}_{12}$ , hereinafter it is marked as YIG) is of particular interest due to its low magnetic and dielectric losses, high electrical resistivity, and stable magnetization [1]. Tailoring its properties via cation substitution, especially with rare-earth elements such as gadolinium, provides an effective strategy for tuning magnetic behaviour and enhancing performance under varying conditions. However, the properties of Gd-doped YIG ferrites strongly depend on both dopant concentration and synthesis route. In this context, developing reliable synthesis approaches that ensure high chemical homogeneity and controlled phase formation is critical for obtaining materials with optimized microwave characteristics.

Yttrium-gadolinium iron garnets ( $\text{Y}_{3-x}\text{Gd}_x\text{Fe}_5\text{O}_{12}$ ,  $x = 0-1.0$ ) were investigated to clarify the mechanisms of garnet phase formation and the influence of gadolinium doping on structural and magnetic properties. The powder materials were synthesized by co-precipitation in aqueous solution followed by thermal treatment up to 1200°C and sintering for ceramic samples at 1400°C.

X-ray diffraction (XRD) and FTIR analysis showed that garnet structure forms via a two-stage mechanism involving an intermediate orthorhombic perovskite phase. At 700-800 °C, yttrium-iron and gadolinium-iron perovskites form, followed by the formation of (Y,Gd)FeO<sub>3</sub>, which reacts with Fe<sub>2</sub>O<sub>3</sub> to yield the garnet phase. Single-phase cubic garnet was obtained at 1200 °C for all compositions [2].

It was found that gadolinium substitution reduces the temperature of garnet formation by ~100 °C, reaching up to 200 °C for selected compositions ( $x = 0.4$  and 1.0). This effect is non-monotonous, indicating a complex role of dopant concentration. In particular, garnet formation occurs at 800 °C for  $x = 0.4$  and already at 700 °C for  $x = 1.0$  [2].

The structural evolution significantly affects ceramic properties. Increasing Gd content leads to reduced porosity, with values below 5% for  $x \geq 0.6$  at relatively low sintering temperatures. Magnetic measurements revealed a non-monotonous variation of saturation magnetization, coercivity, and ferromagnetic resonance linewidth, with an optimum at  $x = 0.6$  [2]. These results demonstrate that Gd doping enables effective control of phase formation, microstructure, and magnetic properties, providing a pathway for designing low-porosity ferrites with the garnet structure with enhanced microwave performance.

---

**KEYWORDS:** YIG garnets, Phase transformation processes, Ceramics, Magnetization saturation, Ferromagnetic resonance linewidth

---

**ACKNOWLEDGEMENTS:** This work was supported by the NAS of Ukraine (grant No 0126U002719 in the framework of the Target Program “Grants of the NAS of Ukraine to research laboratories/groups of young scientists of the NAS of Ukraine” (2026-2027)).

---

### REFERENCES

- [1] E. J. J. Mallmann, A. S. B. Sombra, J. C. Goes, and P. B. A. Fechine, “Yttrium Iron Garnet: Properties and Applications Review”, *Solid State Phenom.*, 202, 65-96 (2013).
- [2] Yu. Shlapa, L. Kovalenko, I. Lisovskyi, V. Zamorskyi, V.-A. Maraloiu, A. Tovstolytkin, M. Popov, H. Chumak, and A. Belous, “Structure Formation and Physical Properties of Gd-Doped Yttrium-Iron Ferrites: Nonlinear Concentration-Temperature Effects and Phase-Dependent Magnetic Behaviour”, *Ceram. Int.*, 52, 6277-6290 (2026).

## Fabrication of the artificial magnetic system and controlling its magnetization states

I. Vetrova<sup>1\*</sup>, J. Šoltýs<sup>2</sup>, J. Tóbiš<sup>2</sup>, J. Feilhauer<sup>2</sup>, S. Sousani<sup>2</sup>, T. Scepka<sup>2</sup>

1) Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská cesta 9, 84104 Bratislava, Slovakia

2) Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava, Slovakia

\* iuliiia.vetrova AT savba.sk

The development of technology has made it possible to fabricate artificial structures at sub-micrometer scales with high precision. In applied magnetism, there is significant research into structurally periodic arrays of magnetic elements. The domain structure is influenced by nearest-neighbor interactions, which are dictated by the sample geometry[1]. There are numerous reasons for difficulties in achieving magnetic order. The main obstacle is the presence of many local minima and large energy barriers among them. The energy barriers are usually much higher than the achievable thermal energy.

In this research, we investigate a square lattice with a ferrotoroidal ground state, characterized by closed magnetization loops within each unit cell. Our goal is to create an array of thin, sub-micron ferromagnetic squares, each divided into four isosceles triangles separated by 30 nm gaps, using precise electron-beam lithography and a lift-off process for permalloy. Before, unidirectional edge states were predicted to exist in such crystals [2]. The magnetic states of the prepared structures are investigated by using a magnetic force microscope.

We can manipulate the magnetization within these elements by applying a local external magnetic field using an MFM probe with a specific magnetic moment in lithography mode. By applying a perpendicular external magnetic field, these changes in magnetic states can be reversed to the ferrotoroidal state. This possibility makes such structures promising for future data processing applications, potentially advancing information storage and manipulation.

---

**KEYWORDS:** MFM, EBL, Micromagnetism, Magnonics, Spin ice

---

**ACKNOWLEDGEMENTS:** We kindly acknowledge support for this work from the VEGA agency, grant number VEGA-2/0167/26

---

### REFERENCES

- [1] J. Lehmann, A. Bortis, P.M. Derlet, C. Donnelly, N. Leo, L.J. Heyderman, M. Fiebig, Relation between microscopic interactions and macroscopic properties in ferroics. *Nature nanotechnology*, 15(11), 896-900 (2020).
- [2] J. Feilhauer, M. Zelent, Z. Zhang, J. Christensen, M. Mruczkiewicz, Unidirectional spin-wave edge modes in magnonic crystal. *APL Materials*, 11(2) (2023).

## Spike-timing-dependent plasticity in artificial “neurons” based on antiferromagnetic spin Hall oscillator for pattern recognition

I. Sotnyk<sup>1</sup>\*, O. V. Prokopenko<sup>1</sup>

1) Taras Shevchenko National University of Kyiv, Ukraine

\* irasotnyk.49 AT gmail.com

The development of next-generation computing systems is increasingly drawing on the principles of biological information processing. Unlike conventional computers, which rely on sequential execution of commands and centralized memory, biological neural networks operate in an ultra-fast and energy-efficient manner, utilizing local learning rules such as Spike-Timing-Dependent Plasticity (STDP). Replicating these biological properties requires physical devices that can mimic the dynamic behavior of real neurons. Artificial “neurons” based on magnetic materials, particularly those that utilize antiferromagnetic (AFM) spin Hall oscillators (SHOs) [1], have recently emerged as promising candidates for neuromorphic computing. These AFM-based “neurons” are capable of generating ultrafast spikes lasting a few picoseconds, exhibit intrinsic plasticity, and can reproduce key neural functions, including spiking activity and response latency [1]. In this work, we build upon a previously proposed programmable AFM-“neuron” (“P-neuron”), which is a simple two-layer neural network consisting of several single-input AFM-“neurons” [2, 3]. Unlike supervised learning approaches, which dominate conventional machine learning [4], our system employs a biologically plausible unsupervised learning scheme based on STDP, allowing the network to self-organize and perform pattern recognition without external labels [2, 4].

We consider the task of unsupervised learning for pattern recognition of binary images using the extended proposed “P-neuron” architecture [2]. In the system, the input symbol is represented as a 5×5 binary image, where each pixel corresponds to a separate AFM-based “neuron”. Each such “neuron” is implemented as a Pt/NiO/Pt spin Hall oscillator driven by direct and alternating current applied to a single Pt contact of the spintronic system [1, 5]. This dynamic generates an output spin current spike that propagates through the second Pt layer, where it is converted into an electrical signal.

The coding of input symbols is performed by converting a binary image into a sequence of time-encoded spikes generated by the first input layer of the “P-neuron”. For unsupervised learning, we employ the Spike-Timing-Dependent Plasticity rule, a biological mechanism that modulates synaptic weights according to the relative timing of pre-synaptic and post-synaptic spikes. Simulation results confirm the effectiveness of the proposed approach. Symbols with simple geometric structures (L, T, U, etc.) are recognized with the highest accuracy, reaching up to 90%. More complex symbols containing closed loops and curved features (B, G, R, etc.) are recognized with an accuracy of 75-80%.

We believe that the “P-neuron” with unsupervised learning is effective at rapidly recognizing small-scale images. Although scaling to larger inputs requires further investigation, results highlight the approach’s potential for energy-efficient neuromorphic computing.

---

**KEYWORDS:** Spin Hall oscillator, Unsupervised learning, Spike-timing-dependent plasticity, Pattern recognition, Neural network

---

**ACKNOWLEDGEMENTS:** This work was supported in part by grant No. 2025.07/0237 from the National Research Foundation of Ukraine. The authors thank all brave defenders of Ukraine who made it possible to finalize this publication.

---

### REFERENCES

- [1] R. Khymyn, I. Lisenkov, J. Voorheis, O. Sulymenko, O. Prokopenko, V. Tiberkevich, J. Akerman, A. Slavin, “Ultra-fast artificial neuron: generation of picosecond-duration spikes in a current-driven antiferromagnetic auto-oscillator,” *Sci. Rep.*, vol. 8, p. 15727, October 2018.
- [2] I. Sotnyk, O. Prokopenko, “Antiferromagnetic Programmable Neuron: Structure, Training, and Pattern Recognition Applications”, *IEEE Journal on Exploratory Solid-State Computational Devices and Circuits*, vol. 12, p. 9, January 2026, DOI:10.1109/JXCDC.2025.3633490.
- [3] H. Bradley *et al.*, “Artificial neurons based on antiferromagnetic autooscillators as a platform for neuromorphic computing,” *AIP Adv.*, vol. 13, no. 1, January 2023, Art. No. 015206.
- [4] H. Bradley, S. Louis, A. Slavin, and V. Tyberkevych, “Pattern recognition using spiking antiferromagnetic neurons,” *Sci. Rep.*, vol. 14, no. 1, September 2024, Art. no. 22373.
- [5] O. Sulymenko, O. Prokopenko, I. Lisenkov, J. Åkerman, V. Tyberkevych, A.N. Slavin, R. Khymyn, “Ultra-fast logic devices using artificial “neurons” based on antiferromagnetic pulse generators,” *J. Appl. Phys.*, vol. 124, p. 152115, September 2018.

## Fabrication and FMR characterization of YIG pellets using cold isostatic pressing for mmWave applications

İ. Yarıcı<sup>1\*</sup>, F. D. Eliçatal<sup>1</sup>, Y. Ozturk<sup>2</sup>

1) *Aydin Adnan Menderes University, Turkey*

2) *Department of Electrical and Electronics Engineering, Faculty of Engineering, Ege University, İzmir, Turkey*

\* yariciismail AT gmail.com

Yttrium iron garnet ( $Y_3Fe_5O_{12}$ , YIG) is a widely used soft ceramic material with unique magnetic and magneto-optical properties, making it highly attractive for optical and microwave applications[1]. Owing to these properties, YIG has been extensively utilized in devices such as circulators, optical isolators, Faraday rotators, phase shifters, switching circuits, antennas, and sensors. Although the magnetic properties of YIG at GHz frequencies are known to depend on both frequency and applied magnetic field, existing studies predominantly focus on YIG spheres and thin films [2]. However, spheres are not suitable for planar structures, while thin films require complex and costly fabrication processes and substrates that may influence magnetization dynamics.

Here, we demonstrate that YIG disk (pellet) structures fabricated using the Cold Isostatic Press (CIP) method provide an effective planar alternative, and their ferromagnetic resonance (FMR) characteristics are investigated in the 4-9 GHz frequency range. The fabrication process includes sol-gel synthesis of YIG powders, uniaxial pressing to form green pellets, CIP processing at 15.000 psi, and subsequent heat treatment. The structural and microstructural properties of the powders and pellets are characterized using X-ray diffraction (XRD), while their magnetic properties are analyzed via vibrating sample magnetometry (VSM). The crystallite sizes of the powders and pellets are found to be 29 nm and 41 nm, respectively, with corresponding saturation magnetization values of 14.5 emu/g and 18.5 emu/g. For FMR characterization, a custom vector network analyzer-based FMR (VNA-FMR) measurement system is developed. Measurements are performed in the 0-3500 G magnetic field range with 500 G increments, and the field-dependent resonance frequencies are obtained. A linear correlation between the resonance frequency and the FMR linewidth was observed, and the gyromagnetic ratio is determined as 2.4 MHz/G, indicating the high magnetic field sensitivity of the material. Our results suggest that CIP-fabricated YIG disks offer a cost-effective and scalable approach for developing sensitive planar microwave devices and integrated magnetic sensors

---

**KEYWORDS:** Cold isostatic press, YIG, Gyromagnetic ratio, FMR characterization, FMR linewidth

---

### REFERENCES

- [1] N. Askarzadeh, H. Shokrollahi. "Microwave device engineering with YIG materials." *Journal of Applied Physics*, 138.22 (2025).
- [2] Bhoi, Biswanath, and Sang-Koog Kim. "Roadmap for photon-magnon coupling and its applications." *Solid State Physics*. Vol. 71. Academic Press,39-71 (2020).

## Microwave absorbing properties of nickel-zinc ferrite and carbonyl iron nanoparticles composites

V. Kukhar<sup>1</sup>, M. Popov<sup>2\*</sup>, O. P. Fedorchuk<sup>3</sup>, T. O. Plutenko<sup>3</sup>, H. Chumak<sup>4</sup>, A. Belous<sup>3</sup>

1) V.I. Vernadsky Institute of General and Inorganic Chemistry, Ukraine

2) Educational and Scientific Institute of High Technologies, Taras Shevchenko National University of Kyiv, Ukraine

3) V. Vernadsky Institute of General and Inorganic Chemistry, NAS of Ukraine, Ukraine

4) Taras Shevchenko National University of Kyiv, Ukraine

\* maxim\_popov AT univ.kiev.ua

With the drastically increasing number of devices with wireless internet access, such as cell phones, IoT systems, etc, the problem of electromagnetic pollution of the environment is only growing. Absorbing materials that decrease the magnitude of electromagnetic radiation can be the principal solution for this problem [1, 2]. Many sensitive to electromagnetic radiation systems require either shielding or coating with absorbing materials that convert external microwave electromagnetic radiation into heat, which is conceptually more rational than shielding. Among the variety of materials tested for microwave absorption, a special place belongs to magnetic dielectrics (ferrites) with high internal dielectric and/or magnetic losses [3, 4]. Here we have synthesized the nanoparticles of nickel-zinc ferrite (NZFO), prepared the polymer-based composite material with variable proportions of NZFO and carbonyl iron (Fe) nanoparticles, and investigated its absorption properties in the 7-18 GHz frequency band. We found that Fe-rich compositions have larger dielectric permittivity (both real  $\epsilon'$  and imaginary  $\epsilon''$  parts) than NZFO-rich samples; however, samples with a large NZFO content exhibit higher values of imaginary permeability  $\mu''$  in the lower part of the investigated band ( $\approx 7-11$  GHz). The absorption properties of composite materials (described by attenuation constant  $\alpha$ ) show that for Fe-rich composition,  $\alpha$  strongly increases with frequency. For NZFO-rich composite  $\alpha$  noticeably decreases and magnetic losses dominate over dielectric. Our results demonstrate that such parameters as  $\epsilon'$ ,  $\epsilon''$ , and  $\mu''$  can be tuned within a certain range by varying the proportion between NZFO, Fe, and polymer. Moreover, the frequency dispersion of the attenuation constant can also be adjusted according to the specific demands (e.g., growing, descending or frequency independent). This research could serve as the starting point in the search for absorbent composite materials to reduce electromagnetic pollution in the microwave frequency range, in view of the forthcoming global deployment of 5G networks.

**KEYWORDS:** Nickel-zinc ferrite nanoparticles, Carbonyl iron, Attenuation constant, X-band, Ku-band

### REFERENCES

- [1] S. K. Dhawan, A. P. Singh, A. Ohlan, K. S. Kakran, and P. Sambyal, Smart Materials Design for Electromagnetic Interference Shielding Applications. Singapore: Bentham Science Publishers, 2022.
- [2] M. Rouhi, Z. Hajizadeh, R. Taheri-Ledari, A. Maleki, and M. Babamoradi, “A review of mechanistic principles of microwave absorption by pure and composite nanomaterials,” Materials Science and Engineering B, vol. 286, pp. 116021, December 2022.
- [3] A. Houbi, A. Zharmenov. Aldashevich, Y. Atassi, Z. Bagasharova Telmanovna, S. Mirzalieva, and K. Kadyrakunov, “Microwave absorbing properties of ferrites and their composites: a review”, Journal of Magnetism and Magnetic Materials, vol. 529, p. 167839, July 2021.
- [4] A. Belous, S. Solopan, V. Kukhar, and M. Popov, “Composite microwave absorbing materials with magnetic constituents: state-of-the-art and possible ways for improving their parameters”, Advanced Engineering Materials, vol. 28, pp. e202502088, February 2026.

## Thermal performance analysis of Fe<sub>3</sub>O<sub>4</sub> nanoparticles under combined AC and DC magnetic fields

Z. Onat<sup>1</sup>\*, E. N. Savranguler<sup>2</sup>, C. Harmansah<sup>3</sup>, Y. Ozturk<sup>1</sup>

1) Department of Electrical and Electronics Engineering, Faculty of Engineering, Ege University, İzmir, Turkey

2) Other, Turkey

3) Ege University, Turkey

\* zeynep.onat.eng AT gmail.com

Magnetic hyperthermia has emerged as an innovative modality for cancer therapy, aiming at selectively destroying tumor cells by generating localized heat under an alternating magnetic field (AMF). Consequently, the use of magnetic nanoparticles (MNPs) in biomedical applications has become more common. Researchers have studied various parameters ranging from particle geometry and chemical composition to magnetic anisotropy and colloidal stability are extensively investigated to optimize heating efficiency and to characterize the performance of MNPs [1,2,3]. In these experiments, an alternating current (AC) magnetic field is mainly employed because it can generate heat; however, the frequency and amplitude must be optimized to avoid affecting healthy tissues. Although studies exist regarding the formation of nanoparticle chain structures under direct current (DC) magnetic fields, there is still limited research on how static external fields interact with an AC field [4,5]. Analyzing the impact of magnetic moment orientation changes under combined AC and DC fields is a fundamental requirement for optimizing magnetic hyperthermia methods.

In this study, measurements were conducted using a specialized magnetic hyperthermia system operating at approximately 88 kHz. A static DC magnetic field, ranging from 0 to 50.8 mT, was applied perpendicular to the AC field. The commercial EFH-1 magnetic fluid, containing Fe<sub>3</sub>O<sub>4</sub> nanoparticles with an average size of 11.6 nm dispersed in a light hydrocarbon, served as the test medium. At an AC field intensity of 0.9 kA/m, the Specific Loss Power (SLP) values decreased from 0.32 W/g to 0.12 W/g as the external DC field strength increased. This reduction is attributed to nanoparticle clustering and chain structure formation induced by the external field, which negatively impacts thermal efficiency.

---

**KEYWORDS:** Magnetic hyperthermia, Magnetic nanoparticles, Fe<sub>3</sub>O<sub>4</sub>, Specific loss power

---

### REFERENCES

- [1] P. Wróblewski, M. Wieteska, M. Midura, G. Domański, D. Wanta, W. Obrębski, .. & Bogorodzki, P. (2026). Analysis of the Feasibility of Concurrent Application of Magnetic Nanoparticles as MRI Contrast Agents and for Magnetic Hyperthermia. *Journal of Functional Biomaterials*, 17(1), 54.
- [2] E.N. Savrangüler, S. Gümüş, C. Harmansah, Y. Öztürk, H. Magat, (2025, September). A Study on the Influence of Magnetic Nanoparticle Concentration on Heating Efficiency in Magnetic Hyperthermia. In 2025 IEEE 15th International Conference Nanomaterials: Applications & Properties (NAP) (pp. NMP07-1). IEEE.
- [3] X. Yu, R. Yang, C. Wu, B. Liu, W. Zhang, The heating efficiency of magnetic nanoparticles under an alternating magnetic field. *Scientific Reports*, 12(1), 16055 (2022).
- [4] C.M. Lucaciu, S. Nitica, I. Fizesan, L. Filip, L. Bilteanu, C. Iacovita, Enhanced magnetic hyperthermia performance of zinc ferrite nanoparticles under a parallel and a transverse bias DC magnetic field. *Nanomaterials*, 12(20), 3578 (2022).
- [5] Nuñez-L. Magos, Lira-J. Escobedo, Rodríguez-R. López, Muñoz-M. Navia, Castillo-F. Rivera, Viveros-P.X. Méndez, ... & Aranda-Espinoza, S. (2021). Effects of DC magnetic fields on magnetoliposomes. *Frontiers in Molecular Biosciences*, 8, 703417.

## Suprising role of Au in crystal growth and physical properties of FeRh single crystals

N. Subotic<sup>1</sup>\*, M. Takahashi<sup>2</sup>, T. Mochiku<sup>3</sup>, Y. Matsushita<sup>4</sup>, T. Kashiwagi<sup>2</sup>, O. Takeuchi<sup>2</sup>, H. Shigekawa<sup>2</sup>,  
K. Kadowaki<sup>2</sup>

1) Co-Creation Institute for Advanced Materials, Shimane University, Japan

2) University of Tsukuba, Japan

3) National Institute for Materials Sciences (NIMS), Japan

4) National Institute for Material Sciences, Japan

\* nikolasubotic95 AT gmail.com

FeRh alloy has captivated researchers for more than 80 years due to its peculiar first-order antiferromagnetic (AFM) to ferromagnetic (FM) transition near room temperature, whose origin is still debated. Additionally, FeRh is regarded as one of the most efficient magnetocaloric materials [1,2]. Despite its interest for both fundamental physics and practical applications, growing high-quality single crystals has been difficult due to the complicated FeRh phase diagram.

In this talk, we present recent results on the single-crystal growth of FeRh using an AuPb flux [3]. We found that Au plays a dominant role in the crystal growth, while Pb reduces the melting temperature. During growth, Au-doped, Rh-doped, near-stoichiometric, and Fe-doped FeRh single crystals were obtained. A first-order AFM-FM transition was observed in the Au-doped and Rh-doped samples. In contrast, different phase transitions occurred in the Fe-doped and near-stoichiometric single crystals. Based on these findings, we propose an origin for the first-order AFM-FM transition.

---

**KEYWORDS:** FeRh single crystals, First order AFM-FM transition, AuPb flux

---

**ACKNOWLEDGEMENTS:** This abstract is supported by the CROSS lab, part of a research proposal: Magnetic and crystal structure analysis of FeRh single crystals, Proposal No. 2023B0151 and Ministry of Education, Science and Innovation of Montenegro, Grant No. 04-082/23-2529/1

---

### REFERENCES

- [1] R. R. Gimaev, A. A. Vaulin, A. F. Gubkin, and V. I. Zverev, Phys. Met. Metall. 121, 823 (2020).
- [2] L. H. Lewis, C. H. Marrows, and S. Langridge, J. Phys. D 49, 323002 (2016).
- [3] N. Subotić, M. Takahashi, T. Mochiku, Y. Matsushita, T. Kashiwagi, O. Takeuchi, H. Shigekawa, and K. Kadowaki Phys. Rev. Materials 8, 023401 (2024).

## Ga<sup>+</sup> focused ion beam impact on Permalloy/Ti/Si heterostructure

S. Krylov<sup>1</sup>, I. Piš<sup>1</sup>, M. Precner<sup>1</sup>, J. Šoltýs<sup>1</sup>, T. Kalmykova<sup>1</sup>, T. Ščepka<sup>1</sup>, S. Sousani<sup>1</sup>, P. Bokes<sup>2</sup>, V. Cambel<sup>1\*</sup>

1) Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava, Slovakia

2) Faculty of Electrical Engineering and Information Technology, Slovak University of Technology in Bratislava, Slovakia

\* Vladimír.Cambel AT savba.sk

This work reports on the quantitative characterisation of the Permalloy/Ti/Si heterostructure after a focused-ion-beam (FIB) milling process used to fabricate magnetically insulated nanostructures. Such structures are needed for high-frequency and magnonic devices [1].

FIB milling has become a standard route for direct-write nanoscale fabrication and local material modification, especially when rapid prototyping or shape flexibility is required. The results show that Ga<sup>+</sup>-FIB can degrade magnetism not only by removing material but also by altering its composition [2,3]. However, a detailed study of the processes involved in FIB processing of magnetic nanostructures remains lacking.

The interaction of the beam with the sample is a complex process due to the high-energy Ga<sup>+</sup> ions (30 keV). The complex interaction includes multiple scattering, electromagnetic interactions, element ionisation, thermal heating, vacancy creation, element diffusion, milling, redeposition, recrystallisation, channelling, etc. The processes are strongly dependent on the Ga<sup>+</sup> dose and sample composition.

To simplify the picture, the processes result in **surface changes** (increased surface roughness, redeposition, and recrystallisation) and **bulk changes** expressed by element redistribution in the heterostructure. In our work, we study surface roughness and redeposition by atomic force microscopy (AFM) and element distribution by X-ray photoelectron spectroscopy (XPS). We compare the results with those from FIB modelling using TRIM and SDTrimSP calculations. A steady-state macroscopic model is used to estimate the evolution of the sample temperature. We explain several features of the XPS and AFM data and show the strong impact of surface damage on bulk element distribution. We discuss in detail some discrepancies that remain between the experiment and the model data.

---

**KEYWORDS:** Magnetic structures, Focused ion beam, XPS

---

**ACKNOWLEDGEMENTS:** We kindly acknowledge support for this work from the VEGA agency, grant number VEGA-2/0167/26.

---

### REFERENCES

- [1] B. Flebus *et al.*, “The 2024 magnonics roadmap,” *J. Phys. Condens. Matter*, vol. 36, no. 36, p. 363501, Sep. 2024, doi: 10.1088/1361-648X/ad399c.
- [2] D. Ozkaya L, R. M. Langford, W. L. Chan, and A. K. Petford-Long, “Effect of Ga implantation on the magnetic properties of permalloy thin films,” *J. Appl. Phys.*, vol. 91, no. 12, pp. 9937-9942, Jun. 2002, doi: 10.1063/1.1477265.
- [3] S. Krylov, T. Kalmykova, T. Ščepka, and V. Cambel, “Magnetic nanostructures with defined magnetic states fabricated by focused ion beam,” *Results Phys.*, vol. 60, p. 107669, May 2024, doi: 10.1016/j.rinp.2024.107669.

## Shape-dependent hybrid acoustic modes in $\text{Ni}_{80}\text{Fe}_{20}$ nanodot phononic crystals

B. Rana<sup>1\*</sup>, P. Graczyk<sup>2</sup>, B. M. Kumar<sup>3</sup>, M. Krawczyk<sup>4</sup>, A. Barman<sup>3</sup>

1) Institute of Spintronics and Quantum Information, Faculty of Physics and Astronomy, Adam Mickiewicz University, Poznan, Poland

2) Institute of Molecular Physics, Polish Academy of Sciences, Poland

3) Department of Condensed Matter and Materials Physics, Satyendra Nath Bose National Centre for Basic Sciences, India

4) Department of Physics of Nanostructures, Adam Mickiewicz University, Poznań, Poland

\* bivran AT amu.edu.pl

In recent years, the surface acoustic waves [1] (i.e., acoustic phonons) have emerged as one of the promising candidates for developing next-generation wave-based information and computation technology. For designing practical devices, it is essential to tailor the frequency versus wavevector characters (i.e., band structures) of acoustic phonons. This can be achieved by patterning artificial crystals on thin films, known as phononic crystals, consisting of periodic arrays of nanoelements or nanodots. On one hand, the dispersion characters of propagating acoustic waves can be controlled by varying the periodicity of the nanodot arrays [2, 3]. On the other hand, the dispersion characters of the localized phonons confined within the nanodots can be tuned through the dot geometry. This offers a unique route to tailor the phononic band structure and enable the coupling between localized and propagating phonon modes. Such phonon-phonon coupling is crucial for realizing novel device functionalities, including intermode energy transfer.

In this work, we study femtosecond pulsed laser-induced acoustic phonons in phononic crystals by employing an all-optical pump-probe technique [4]. The phononic crystals are made of 50-nm-thick Py ( $\text{Ni}_{80}\text{Fe}_{20}$ ) elements with three different shapes: rectangular, diamond, and elliptical. The nanodots, each having lateral dimensions of 200 nm × 250 nm, are periodically arranged in a square lattices on a Si/SiO<sub>2</sub> substrate with varying lattice constant from 275 to 600 nm. The experimental results are corroborated with finite element method-based numerical simulations. Several propagating phononic modes, namely Rayleigh-type surface acoustic waves, are observed in all the phononic crystals. Their frequencies are found to increase linearly with the inverse of the lattice constant. We also identify phononic modes localized within the nanodots, whose frequencies vary with the dot shape. Interestingly, strong coupling between propagating and localized phononic modes are observed in arrays of diamond-shaped nanodots, resulting in the emergence of a high-intensity hybrid phononic mode. The coupling becomes weaker for arrays of elliptical dots. In contrast, no mode coupling is observed in arrays of rectangular nanodots, where the propagating and localized phonons modes remain well separated in frequency. We believe that the ability to control propagating phonons with lattice periodicity and to optimize their coupling with localized phonons via nanodot shape engineering opens exciting opportunities for the realization of advanced phononic devices for wave-based signal processing, energy transfer, and on-chip information technologies.

**KEYWORDS:** Metallic nanodot arrays, Time-resolved magneto-optical Kerr effect (TR-MOKE) microscopy, Acoustic phonons, Mode coupling, Numerical simulations

**ACKNOWLEDGEMENTS:** BR acknowledges NCN SONATA-16 project (Grant no. 2020/39/D/ST3/02378). AB gratefully acknowledges the financial support from Department of Science and Technology, Government of India under Grant Nos. SR/NM/NS-09/2007 and INT/JP/JST/P-23/09.

### REFERENCES

- [1] L. Hackett, M. Miller, F. Brimigion, D. Dominguez, G. Peake, A. Tauke-Pedretti, S. Arterburn, T. A. Friedmann, and M. Eichenfield, Towards single-chip radiofrequency signal processing via acoustoelectric electron-phonon interactions, *Nat. Commun.* 12, 2769 (2021).
- [2] P. Graczyk, B. Rana, A. Trzaskowska, B. K. Mahato, J. W. Kłos, M. Krawczyk, and A. Barman, Optical excitation and detection of high-frequency Sezawa modes in Si/SiO<sub>2</sub> system decorated with Ni<sub>80</sub>Fe<sub>20</sub> nanodot arrays, *Ultrasonics* 148, 107522 (2025).
- [3] A. Comin, C. Giannetti, G. Samoggia, P. Vavassori, D. Grandi, P. Colombi, E. Bontempi, L. E. Depero, V. Metlushko, B. Ilic, and F. Parmigiani, Elastic and magnetic dynamics of nanomagnet-ordered arrays impulsively excited by subpicosecond laser pulses, *Phys. Rev. Lett.* 97, 217201 (2006).
- [4] B. Rana, D. Kumar, S. Barman, S. Pal, Y. Fukuma, Y. Otani, and A. Barman, Detection of picosecond magnetization dynamics of 50 nm magnetic dots down to the single dot regime, *ACS Nano* 5, 9559 (2011).

## When Curie-weiss theory breaks down: Unified description of size- and shape-dependent Curie-weiss behaviour in nanomagnets

S. Nqayi<sup>1</sup>\*, L. L. Noto<sup>2</sup>

1) Department of Physics, University of the South Africa, P.O. Box 392, Florida Campus, South Africa, South Africa

2) University of South Africa, South Africa

\* sbunqayi AT gmail.com

The classical Curie-Weiss law successfully describes magnetic susceptibility in bulk materials; however, its assumptions of homogeneity and infinite size become invalid at the nanoscale, where surface disorder, reduced atomic coordination, and shape anisotropy strongly influence magnetic behaviour. In this work, we present a geometry-dependent modification of the Curie-Weiss equation that incorporates finite-size effects through explicit separation of surface and core magnetic contributions. A surface fraction parameter,  $\eta$ , is introduced to quantify morphology-dependent magnetic inhomogeneity in nanoscale systems. Analytical formulations are derived for spherical and cubic nanostructures, demonstrating how particle size and geometry renormalise both the Curie constant and Weiss temperature. The model predicts a systematic crossover from surface-dominated magnetic disorder in ultrasmall particles to bulk-like Curie-Weiss behaviour with increasing particle dimensions, while naturally recovering the classical thermodynamic limit. The proposed framework provides a physically transparent and generalised mean-field description of magnetic susceptibility in finite systems, establishing particle size and morphology as key control parameters for nanoscale magnetic order. These results offer new insight into the design and optimisation of functional magnetic nanomaterials for advanced technological applications.

---

**KEYWORDS:** Finite-size effects, Magnetic nanomaterials, Modified Curie-Weiss law, Surface-to-volume ratio, And shape anisotropy

## Symmetry-dependent resonances in Fe/MgO/ZnO/MgO/Fe sandwiches

S. Chakraborti<sup>1</sup>\*, A. Sharma<sup>2</sup>

1) Indian Institute of Technology Ropar, India

2) IIT Mandi, India

\* sabarna.20eez0025 AT iitrpr.ac.in

Following the pioneering study on Fe/MgO/Fe sandwiches [1], two decades have been devoted to discover materials that simultaneously enhance spin-transfer torque (STT) and tunnel magnetoresistance (TMR) for faster, energy-efficient switching with improved readability in high-performance magnetic tunnel junctions (MTJs). Even when fabrication challenges are set aside, theoretical efforts have consistently fallen short of delivering the desired outcomes. MgO, owing to the symmetry-dependent tunnelling of the  $\Delta_1$  states, has retained its position as the preferred tunnel barrier for foundry-grade MTJs. However, the physics of single-barrier tunnelling in MgO imposes an intrinsic trade-off between the TMR and the RA product in conventional MTJs. To address this issue of regular tunnelling, we explore the physics of symmetry-driven resonances of the  $\Delta_1$  states [2] in a magnetic tunnel junction (MTJ) comprising an Fe(001)/MgO(001)<sub>2-layers(1)</sub>/ZnO(001)<sub>31</sub>/MgO(001)<sub>21</sub>/Fe(001) heterostructure, premised on the self-consistent coupling of the non-equilibrium Green's function (NEGF) with density functional theory (DFT). The conceived heterostructure-based MTJ, titled  $\Delta_{1R}$ -MTJ, opens up a new frontier for engineering high-performance MTJs, providing a sizable tunnel magnetoresistance (TMR) of  $\approx 6 \times 10^3$  % and a nominal resistance-area (RA) product of 0.14  $\text{fi} \cdot \mu\text{mZ}$ , with a high ( $\approx 99\%$ ) spin polarisation. The TMR% observed here is  $\approx 3.2$  times higher, and the RA product is  $\approx 6.5$  times lower than that of a 4L-MgO-based MTJ at zero bias. These attributes indicate a significant enhancement in STT, thereby enabling swift and energy-efficient switching dynamics in the  $\Delta_{1R}$ -MTJ. The quantum well in this system is designed with an insulator, instead of metals, to primarily capitalize on the absence of non- $\Delta_1$  symmetry bands near the Fermi window, and avoid scattering at room temperature that disrupts the resonance. Furthermore, the Fe/MgO/ZnO/MgO/Fe stack in the  $\Delta_{1R}$ -MTJ is compatible with foundry-grade CMOS processing.

**KEYWORDS:** Tunnelmagnetoresistance, Symmetry-dependent resonant tunneling, Spin transfer torque (STT)

**ACKNOWLEDGEMENTS:** The author Abhishek Sharma acknowledges the support by the Science and Engineering Research Board (SERB), Government of India, Grant No. SRG/2023/001327.

### REFERENCES

- [1] Phys. Rev. B 63, 054416 - Published 8 January, 2001
- [2] Symphony of Symmetry Selective Resonances in Fe-MgO-Fe: arXiv:2504.09842 (2025)

## Role of amino acids in tailoring the magnetism of CoFe<sub>2</sub>O<sub>4</sub> nanoparticles

A. Raveendran<sup>1\*</sup>, S. Ramanavičius<sup>1</sup>, A. Drabavicius<sup>2</sup>, V. Pakstas<sup>3</sup>, K. Mazeika<sup>4</sup>, A. Balciunaite<sup>5</sup>, M. Talaikis<sup>6</sup>, A. Mikalauskaite<sup>7</sup>, G. Paulikaite<sup>7</sup>

1) Department of Electrochemical Material Science, State Research Institute Center for Physical Sciences and Technology, Lithuania

2) Department of Structural Analysis of Materials, Center for Physical Sciences and Technology, Vilnius, Lithuania

3) Department of Structural Analysis of Materials, Center for Physical Sciences and Technology, Vilnius, Lithuania

4) Nuclear Research Department, Center for Physical Sciences and Technology, Vilnius, Lithuania

5) Catalysis Department, Center for Physical Sciences and Technology, Vilnius, Lithuania

6) Center for Physical Sciences and Technology (FTMC), Lithuania

7) Department of Electrochemical Material Science, State Research Institute Center for Physical Sciences and Technology (Lithuania), Lithuania

\* aswathi.raveendran AT ftmc.lt

Magnetic nanoparticles exhibit tunable size-dependent physicochemical and magnetic properties, making them attractive for applications in data storage, magneto-optical devices, photocatalysis, and biomedicine [1,2]. Cobalt ferrite (CoFe<sub>2</sub>O<sub>4</sub>) is a technologically important ferrite due to its high magneto crystalline anisotropy, chemical stability, and mechanical hardness. However, its structural and magnetic properties are strongly governed by particle size, morphology, and surface chemistry, which are highly sensitive to synthesis conditions. Established synthesis routes such as hydrothermal, sol-gel, and co-precipitation methods enable modulation of nucleation and growth kinetics through parameters including temperature, pH, and stirring rate [3,4]. Despite these advantages, CoFe<sub>2</sub>O<sub>4</sub> nanoparticles typically exhibit strong agglomeration arising from high surface energy and magnetic dipole interactions, which limits their functional performance. Surface modification using surfactants or capping molecules has been shown to mitigate aggregation through electrostatic and steric stabilization while enabling controlled particle growth and surface functionalization [5].

Herein, CoFe<sub>2</sub>O<sub>4</sub> nanoparticles were synthesized via a hydrothermal co-precipitation route in the presence and absence of amino acids acting as capping agents [1]. The role of amino acid functionalization on crystallographic structure, morphology, and magnetic behaviour was systematically examined. The results demonstrate that amino acid capping significantly enhances nanoparticle dispersion and customize magnetic properties, thereby improving functional performance. These findings suggest that amino acid-modified CoFe<sub>2</sub>O<sub>4</sub> nanoparticles are promising candidates for magnetically recoverable adsorbents and catalytic systems in wastewater treatment.

**KEYWORDS:** Magnetic nanoparticles, Cobaltferrites (CoFe<sub>2</sub>O<sub>4</sub>) nanoparticles, Tuning magnetism, Amino acid surfactants, Environmental remediation

**ACKNOWLEDGEMENTS:** This project received funding from the Research Council of Lithuania (LMTLT), agreement No S-MIP-24-14.

### REFERENCES

- [1] R. Žalnėravičius, A. Mikalauskaitė, G. Niaura, A. Paškevičius, A. Jagminas, “Ultra-small methionine-capped Au<sup>0</sup>/Au<sup>+</sup> nanoparticles as efficient drug against the antibiotic-resistant bacteria”, *Mater Sci Eng:C*, 102, 646-652, (2019).
- [2] A. Raveendran, E. Semasko E, A. Jagminas, A. Sukoviene, S. Ramanavicius, “Current trends in cobalt and zinc ferrite based magnetic photocatalysts for wastewater treatment”, *Inorganic Chemistry Communications*, 183, 115876, (2026).
- [3] A. Sukoviene, S. Ali, A. Jagminas, S. Ramanavicius, “Magnetic Cobalt and Other Types of Ferrite Nanoparticles: Synthesis Aspects and Novel Strategies for Application in Wastewater Treatment”, *Appl. Sci.*, 15(2), 857, (2025).
- [4] M. Plečkaitis, V. Karabanovas, G. Butkiene, J. Venius, M. Burkanas, G. Grinciene, A. Jagminas, R. Rotomskis, “Magnetic Nanoparticles Decorated with Gold Nanoclusters-Applications in Cancer Theranostics”, *Adv. Mater. Interfaces*, 10, 1-12, (2023).
- [5] M. Kurtinaitiene, K. Mazeika, S. Ramanavicius, V. Pakstas, A. Jagminas, “Effect of Additives on the Hydrothermal Synthesis of Manganese Ferrite Nanoparticles”, *Adv. Nano. Res.*, 4, 1-14, (2016).

## Hall effect in $[\text{Fe}/\text{I}]_n$ discontinuous multilayers ( $\text{I} = \text{SiO}_2, \text{MgO}, \text{HfO}_2$ )

I. Pazukha<sup>1</sup>, O. Pylypenko<sup>1</sup>, D. Kabyletskyi<sup>1</sup>, S. Vorobiov<sup>2\*</sup>, V. Komanicky<sup>2</sup>, Y. Shkurdoda<sup>1</sup>

1) Sumy State University, Ukraine

2) Department of Condensed Matter Physics, Faculty of Science, P.J. Šafárik University, Park Angelinum 9, 041 54 Košice, Slovakia

\* serhii.vorobiov AT upjs.sk

The practical interest in nanocomposites stems from their potential for use as magnetosensitive elements in nanoelectronics, spintronics, computing, and other fields [1-3]. The use of such materials enables improved device reliability and significantly reduced size, weight, power consumption, and cost [3-6]. One of the effects utilized in such structures, on which highly sensitive magnetic field sensors, microelectronic compasses, displacement sensors, and rotational speed sensors can be developed, is the Hall effect [7, 8]. Hall sensors are widely used across many areas of modern industry, including mechanical engineering, automotive electronics, aviation technology, welding equipment, medical equipment, household appliances, and computer technology. The transport sector utilizes a wide range of sensors for safety, engine performance monitoring, and vehicle positioning systems [9].

The aim of this work was to conduct an experimental study of the Hall effect in as-deposited and annealed at 700 K  $[\text{Fe}(d)/\text{I}(3)]_{10}/\text{S}$  discontinuous multilayers ( $\text{I} = \text{SiO}_2, \text{MgO}, \text{HfO}_2$ ) obtained by the method of sequential layer magnetron sputtering in a vacuum. The Hall effect was measured at room temperature using a four-point configuration. When measuring the Hall voltage in the case where the vectors of the electric current density and the magnetic field induction are mutually perpendicular, account was taken of the contributions of additional (parasitic) draw arising in the circuit due to secondary thermal and galvanomagnetic effects. To minimize the impact of these negative factors and the asymmetry in contact placement, four measurements were taken with the electric current flowing in different directions in the presence of a magnetic field.

For  $[\text{Fe}(2)/\text{I}(3)]_{10}/\text{S}$  discontinuous multilayers (after annealing at 700 K) and  $[\text{Fe}(7)/\text{I}(3)]_{10}/\text{S}$  discontinuous multilayers (after deposition and annealing at 700 K), regardless of the insulator material, both the anomalous and normal Hall effects are observed. For all structures with  $d_{\text{Fe}} = 7$  nm, the anomalous Hall effect is observed over a wide range of magnetic fields (-2 - +2 T). This makes it possible to use them as sensitive elements in magnetic field sensors that are stable in the presence of various physical fields. For as-deposited and annealed at 700 K  $[\text{Fe}(7)/\text{MgO}(3)]_{10}/\text{S}$  and  $[\text{Fe}(7)/\text{HfO}_2(3)]_{10}/\text{S}$  discontinuous multilayers, the value of the anomalous Hall effect is  $(1.8-4.2) \cdot 10^{-9}$  m<sup>3</sup>/C and is only slightly dependent on the type of dielectric layers and heat treatment. A decrease in the Fe layer thickness to 2 nm results in a 6- to 7-fold increase in the intrinsic Hall coefficient, primarily due to structural changes in the system (the transition to island films).

**KEYWORDS:** Discontinuous multilayers, Magnetron sputtering, Magnetic metal, Insulator, Hall effect

**ACKNOWLEDGEMENTS:** This work was funded by the NATO Program “Science for Peace and Security” (Project No. G6131) and the State Program of the Ministry of Education and Science of Ukraine (Project No. 0224U033036).

### REFERENCES

- [1] M. Mi, H. Xiao, L. Yu, Y. Zhang, Y. Wang, Q. Cao, and Yilin Wang, “Two-dimensional magnetic materials for spintronic devices”, *Materials Today Nano*, 24, 100408 (2023).
- [2] Y. Ma, G. Li, J. Du, M. Li, J. Wang, and Qiang Wang, “Size-dependent structure and magnetic properties of co-evaporated Fe-SiO<sub>2</sub> nanoparticle composite film under high magnetic field”, *AIP Adv.*, 6, 055929 (2016).
- [3] M. Nichterwitz, S. Honnali, J. Zehner, S. Schneider, D. Pohl, S. Schiemenz, S.T.B. Goennenwein, K. Nielsch, and Karin Leistner, “Control of positive and negative magnetoresistance in iron oxide-iron nanocomposite thin films for tunable magnetoelectric nanodevices”, *ACS Appl. Electron. Mater.*, 2, 2543 (2020).
- [4] A. Vovk, A. García-García, Y.G. Pogorelov, J.A. Pardo, P. Štrichovanec, C. Magén, P.A. Algarabel, J.P. Araujo, and G.N. Kakazei, “Probing the morphology of epitaxial Fe/MgO discontinuous multilayers by magnetometric technique”, *J. Magn. Magn. Mater.*, 474, 369 (2019).
- [5] Bao-Huei Huang, Yu-Hsiang Fu, Chao-Cheng Kaun, and Yu-Hui Tang, “Determining perpendicular magnetic anisotropy in Fe/MgO/Fe magnetic tunnel junction: A DFT-based spin-orbit torque method”, *J. Magn. Magn. Mater.*, 585, 171098 (2023).
- [6] J.C. Denardin, M. Knobel, L.S. Dorneles, and L.F. Schelp, “Structural, magnetic and transport properties of discontinuous granular multilayers”, *J. Magn. Magn. Mater.*, 294 206 (2005).
- [7] S. Yenuganti, S.S. Raju, H. Settibhaktini, “A brief review of Hall effect-based sensors”, *Sensor Rev.*, 46, 442 (2026).
- [8] Y. Zhou, F. Priscila, S. Rosa, Jing Guo, Shu Cai, Rong Yu, Sheng Jiang, Ke Yang, Aiguo Li, Qimiao Si, Qi Wu, Zachary Fisk, and Liling Sun, “Hall coefficient diagnostics of the surface state in pressurized SmB<sub>6</sub>”, *Phys. Rev. B*, 101, 125116 (2020).

## Correlation between ferromagnetic resonance and giant magnetoresistance in granular Co-Ag alloy thin films

I. Shpetnyy<sup>1,2,\*</sup>, L. Satrapinsky<sup>1</sup>, V. Hrebynakha<sup>3</sup>, S. Vorobiov<sup>4</sup>, U. Shvets<sup>2</sup>, D. Derecha<sup>3</sup>, Y. Shkurdoda<sup>2</sup>, S. Shvets<sup>2</sup>, T. Kulyk<sup>2</sup>, I. Kozak<sup>5,3</sup>, T. Plecenik<sup>1</sup>

1) Centre for Nanotechnology and Advanced Materials, Faculty of Mathematics, Physics and Informatics, Comenius University Bratislava, Mlynská Dolina, 84248 Bratislava, Slovakia

2) Sumy State University, Kharkivska Str. 116, 40007 Sumy, Ukraine

3) V.G. Baryakhtar Institute of Magnetism of the NAS of Ukraine, Acad. Vernadsky Blvd. 36-b, 03142 Kyiv, Ukraine

4) Department of Condensed Matter Physics, Faculty of Science, P.J. Šafárik University, Park Angelinum 9, 041 54 Košice, Slovakia

5) Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská cesta 9, 84104 Bratislava, Slovakia

\* i.shpetnyy AT gmail.com

The development of magnetic nanomaterials is a key direction for advancing spintronics and nanoelectronics. Of particular interest are granular Co-Ag thin films, in which ferromagnetic nanograins are dispersed in a non-magnetic metallic matrix, giving rise to giant magnetoresistance (GMR) due to spin-dependent scattering of charge carriers at ferromagnetic granule/non-magnetic matrix interfaces and within the ferromagnetic granules themselves [1]. Ferromagnetic resonance (FMR) is an informative technique for probing magnetic nanostructure, effective magnetic fields, and spin dynamics. However, the correlation between GMR and FMR in such systems remains insufficiently understood.

In this work, an experimental study was carried out to establish a correlation between magnetoresistive behavior, dynamic magnetic properties, and structural state of granular  $\text{Co}_x\text{Ag}_{100-x}$  thin films in the as-deposited state. Films with  $15 \text{ at.}\% \leq x \leq 75 \text{ at.}\%$  and a thickness of 85 nm were prepared by electron-beam co-evaporation. The nanostructure was analyzed by TEM, including HRTEM. Transverse and longitudinal magnetoresistance were measured at 140-440 K in magnetic fields up to 1.6 kOe. GMR exhibits pronounced maxima at  $x = 26-32 \text{ at.}\%$ , correlating with the structural percolation threshold. With increasing temperature, the GMR peak shifts from 26 to 32 at.%, indicating a stronger superparamagnetic contribution at lower Co content. A maximum GMR of 1.26% at 1.6 kOe was obtained for  $x = 26 \text{ at.}\%$  at 140 K, decreasing by a factor of 1.3 at 290 K. High-field measurements (up to 90 kOe) for the predominantly superparamagnetic  $x = 26 \text{ at.}\%$  sample revealed a GMR of 33% at 5 K, attributed to suppression of thermal fluctuations and alignment of magnetic moments. FMR spectra show nearly isotropic resonance fields ( $\sim 2 \text{ kOe}$ ) for  $x \leq 26 \text{ at.}\%$ , indicating weak intergranular interactions, whereas for  $x = 75 \text{ at.}\%$  the perpendicular resonance field reaches  $\sim 15 \text{ kOe}$  due to strong anisotropy. This evolution correlates with an increase in effective magnetization from  $\sim 48$  to  $\sim 1000 \text{ emu/cm}^3$ , evidencing a transition from a superparamagnetic granular ensemble to an exchange-coupled ferromagnetic system.

A clear correlation between GMR and FMR characteristics is established, governed by concentration-driven changes in magnetic nanostructure and intergranular interactions.

---

**KEYWORDS:** Ferromagnetic resonance, Giant magnetoresistance, Co-Ag alloy thin films, Percolation threshold, Superparamagnetism

---

**ACKNOWLEDGEMENTS:** This work was supported by the IEEE Magnetics Society (STCU Project No. 9918 "Magnetism in Ukraine Initiative") and the State Program of the Ministry of Education and Science of Ukraine (Project No. 0224U033036).

### REFERENCES

- [1] A.E. Berkowitz, J.R. Mitchell, M.J. Carey, A.P. Young, S. Zhang, F.E. Spada, F.T. Parker, A. Hutten, and G. Thomas, "Giant magnetoresistance in heterogeneous Cu-Co alloys", *Physical Review Letters*, vol. 68, pp. 3745-3748 (1992).

## Mutual synchronization in a three-element antiferromagnetic spin Hall array

O. Shtanko<sup>1\*</sup>, O. V. Prokopenko<sup>1</sup>

1) Taras Shevchenko National University of Kyiv, Ukraine

\* olegshtanko2000 AT gmail.com

The unique properties of antiferromagnetic (AFM) materials facilitate breakthroughs in modern fields, notably ultrafast spintronics and terahertz-frequency (THz) systems. A spin Hall oscillator (SHO) consisting of adjacent AFM and heavy-metal (typically Pt) layers could be a useful platform for promising applications utilizing THz magnetization dynamics [1, 2]. While a single AFM SHO can be frequency-tuned via a DC current, its practical implementation is severely limited by a low output power that usually does not exceed 1  $\mu\text{W}$ . A widely recognized strategy to overcome this limitation is to synchronize multiple oscillators. While dual-oscillator systems are well documented, the complex nonlinear dynamics of larger AFM arrays remains mostly unexplored.

In this paper, we propose and investigate a planar array consisting of three mutually coupled AFM Josephson-like SHOs [3], which could be convenient system for achieving larger output powers than in a single SHO.

We consider a geometry in which three distinct AFM Josephson-like oscillators are situated on top of a common Pt layer. Local DC drive currents in the Pt layer excite THz rotation of magnetization in each AFM region via the spin-orbit torque. The common Pt layer acts as a coupling channel for pure spin currents, providing a symmetric mutual coupling mechanism between the adjacent precessing magnetizations of SHOs.

We numerically solve a system of coupled non-isochronous phase equations governing the AFM Néel vectors and investigate the collective behavior of the three AFM SHOs array for various DC drive currents. To rigorously manage the extreme computational stiffness caused by the intrinsic terahertz-frequency nutations, the numerical integration was executed utilizing adaptive stiffness-switching algorithms. Furthermore, the reliable extraction of the true locking thresholds from the massive parametric sweep necessitated a customized contiguous-block algorithm to explicitly filter out chaotic numerical artifacts generated by transient chimera states. Transient dynamical analysis confirms robust phase-locking between the three elements. The obtained synchronization bandwidth was approximately  $0.024 \times 10^8 \text{ A/cmZ}$ , spanning a drive current window from  $1.988 \times 10^8 \text{ A/cmZ}$  to  $2.012 \times 10^8 \text{ A/cmZ}$ . In addition, by performing an inverse parametric sweep and constructing a high-resolution 2D phase coherence map, we successfully extracted the global synchronization boundaries (Arnold tongue) of the system [4]. Our calculations reveal that the investigated array exhibits unique topological transitions, including a sudden expansion of the synchronization bandwidth at critical coupling strengths of approximately 0.1 due to the overcoming of non-isochronous frequency shifts.

We believe that understanding the observed complex multi-oscillator locking regimes is a crucial step toward the development and optimization of high-power, highly coherent AFM THz signal sources.

---

**KEYWORDS:** Antiferromagnet, Spin Hall oscillator, Terahertz frequency, Mutual synchronization

---

**ACKNOWLEDGEMENTS:** This work was supported in part by grant No. 2025.07/0237 from the National Research Foundation of Ukraine. The authors thank all brave defenders of Ukraine that made finalizing this publication possible.

---

### REFERENCES

- [1] H. Bradley, S. Louis, C. Trevillian, L. Quach, E. Bankowski, A. Slavin, V. Tyberkevych, “Artificial neurons based on antiferromagnetic auto-oscillators as a platform for neuromorphic computing,” *AIP Adv.*, vol. 13, p. 015206, Jan. 2023.
- [2] O. R. Sulymenko, O. V. Prokopenko, V. S. Tiberkevich, A. N. Slavin, B. A. Ivanov, and R. S. Khymyn. “Terahertz-frequency spin Hall auto-oscillator based on a canted antiferromagnet,” *Phys. Rev. Appl.*, vol. 8, no. 6 p. 064007, December 2017.
- [3] R. Khymyn, I. Lisenkov, V. Tiberkevich, B. A. Ivanov, and A. Slavin, “Antiferromagnetic THz-frequency Josephson-like oscillator driven by spin current,” *Sci. Rep.*, vol. 7, no. 1, p. 43705, Mar. 2017.
- [4] A. N. Slavin and V. S. Tiberkevich, “Nonlinear Auto-Oscillator Theory of Microwave Generation by Spin-Polarized Current,” *IEEE Trans. Magn.*, vol. 45, no. 4, pp. 1875-1918, May 2009.

## Time-resolved linear dichroism in magnetic fluids: Concentration-dependent optical response

N. E. Taşçılar<sup>1\*</sup>, Y. Ö. Ömür<sup>1</sup>, E. Kara<sup>2</sup>, Y. Ozturk<sup>1</sup>

1) Department of Electrical and Electronics Engineering, Faculty of Engineering, Ege University, İzmir, Turkey

2) Department of Mechatronics Engineering, Ege University, İzmir, Turkey

\* emirtascilar22 AT gmail.com

Magnetic fluids (ferrofluids) have attracted significant attention due to their unique field-responsive optical properties, enabling applications in photonics, biomedical devices, sensing, and tunable optical components. In particular, linear dichroism, arising from field-induced nanoparticle alignment, offers a promising mechanism for optical switches, sensors, and modulators. However, time-resolved and concentration-dependent studies of dichroic behavior in commercially available ferrofluids remain limited in the literature, especially within the visible spectral range [1, 2]. In this study, we investigate the linear dichroism of a commercial magnetic fluid (EFH<sub>1</sub>) by performing transmission measurements under two orthogonal polarization states in the 500-800 nm wavelength range. The experiments were conducted using a spectrometer (OceanView - USB<sub>4000</sub>) while the ferrofluid sample was placed in a cuvette with a 2-mm optical path between the poles of an electromagnet. Measurements were carried out under applied magnetic fields ranging from 0.19 T to 0.75 T. Measurements were acquired with a temporal resolution of 600 ms, and the ferrofluid concentration varied between 1% and 5%. The results reveal a pronounced polarization-dependent transmission behavior under an applied magnetic field. At 600 nm, a maximum transmission decrease of approximately 20% was observed when the polarization was aligned parallel to the magnetic field, while a reduction of about 10% was measured for the perpendicular polarization. Time-dependent analysis shows that the system reaches equilibrium faster at lower concentrations: the response time was determined to be approximately 3 s for 1% concentration, 4.2 s for %5 concentration with polarization parallel to the applied field. These findings provide new insights into the dynamic optical response of magnetic fluids and highlight their potential for use in fast and tunable magneto-optical devices, such as optical modulators.

---

**KEYWORDS:** Magnetic fluids, Ferrofluids, Linear dichroism, Magneto-optical effects, Time-resolved measurement

---

### REFERENCES

- [1] S. Malynych, I. Moroz, Time dependent magnetically induced variations in optical transmission of magnetite nanoparticle aqueous suspension. *Central European Journal of Physics*, 10(1), 159-165 (2012).
- [2] H. Cui, H. Ma, T. Zhang, X. Jin, Z. Tian, J. Liu, Recent Advances in the Applications of Magnetic Fluids. *NANO* (2026).

## First-principles study of transition metal (Cu, Mo) doped 2d BiOI: Tunable electronic and magnetic properties for spintronic applications

A. Mosbah<sup>1\*</sup>

*1) Laboratory of Studies of Surfaces and Interfaces of Solid Materials, Faculty of Sciences, Setif, Algeria*

\* ammar.mosbah AT usa.com

This paper conducts a detailed first-principles analysis using Density Functional Theory (DFT) to investigate the structural, electrical, and magnetic properties of Cu- and Mo-doped BiOI. The findings show that both dopants maintain the structural stability of the host lattice while significantly altering its physical properties [1]. The electrical structure analysis demonstrates that both Cu and Mo doping cause a semiconductor-to-metal transition, as dopant-induced states cross the Fermi level. However, the nature of these states varies greatly depending on the dopant. Cu doping causes relatively localized 3d states to strongly hybridize with O 2p orbitals, resulting in moderate metallic behavior. In contrast, Mo doping produces more delocalized 4d states with higher multi-orbital hybridization, resulting in increased electrical conductivity and a more prominent metallic character. Spin-polarized computations demonstrate that both systems are magnetically ordered.

Cu-doped BiOI has a net magnetic moment of around 2  $\mu_B$ , which is primarily focused on the Cu atom and mediated by oxygen via super exchange interactions. Mo-doped BiOI, on the other hand, shows greater delocalized magnetic activity, with spin polarization extending across the lattice due to the itinerant nature of Mo 4d electrons.

Comparative analysis highlights the crucial role of d-orbital character in determining the electronic and magnetic properties of doped BiOI.

While Cu doping favors localized magnetism with regulated electronic states, Mo doping promotes increased conductivity and itinerant magnetism. These findings show that selective transition metal doping is an effective way to adjust the functionality of BiOI, making it a promising candidate for spintronic and multifunctional electronics [2].

---

**KEYWORDS:** BiOI, Doping, DFT, Physical properties, Spintonic

---

### REFERENCES

- [1] W. Kohn, L. J. Sham, “Self-consistent equations including exchange and correlation effects,” *Phys. Rev.*, 140, A1133(1965).
- [2] R. M. Martin, “Electronic Structure: Basic Theory and Practical Methods”, Cambridge University Press, (2004).

## Spin-wave implementation within the VAMPIRE software package

S. I. Ruta<sup>1</sup> \*

1) Sheffield Hallam University, United Kingdom

\* sergiu.ruta AT shu.ac.uk

Spin waves, also known as magnons, are collective excitations of the spins in a magnetic material. Spin waves play an important role in the behaviour of magnetic materials, determining the system response in the GHz and THz regimes. The spin-wave dispersion relation, i.e. the spin wave frequencies as a function of the wavevector can be calculated theoretically using both atomistic spin dynamics (ASD) and linear spin wave theory (LSWT). The LSWT is a first-order approximation for the spin-wave dispersion relation and can be computed using the SpinW [1] implementation.

The LSWT is limited by its linear approximation, which restricts it to small oscillations and long-wavelength excitations, and it cannot account for nonlinear effects or finite-temperature spin fluctuations. The ASD overcomes these limitations, simulating individual spins at the atomic level to capture nonlinear behaviour, thermal effects, and localized phenomena in complex magnetic systems. The temperature dependence of spin waves is important for understanding the dynamic properties of a wide range of magnetic materials. In spintronics, THz emission and the spin Seebeck effect are directly related to the SW and magnon-magnon [2] and magnon-phonon [3] interactions.

In this work we will present the implementation of spin-wave calculations into the VAMPIRE software package [4,5]. The ASD model implemented in the current VAMPIRE software is able to describe a large range of temperature-dependent magnetic properties and the dynamics of complex magnetic systems. This allows simulation of spin waves for complex magnetic materials (ferromagnetic, ferrimagnetic, antiferromagnetic and frustrated spin configurations) and various geometries (core-shell particles, multilayers, system with defects/impurities) and 2D materials.

---

**KEYWORDS:** Magnetisation dynamics, Spin wave, Magnons, VAMPIRE

---

### REFERENCES

- [1] <https://www.spinw.org/>
- [2] Z. Shi, *et al.*, PRL, 127(27), (2021).
- [3] Bozhko, *et al.*, Low Temperature Physics, 46(4), (2020).
- [4] R.F. Evans, *et al.*, Journal of Physics: Condensed Matter, 26(10), (2014).
- [5] <https://vampire.york.ac.uk/>

## Rectification of pulse signals in a ferromagnetic spin-torque microwave detector

V. Prokopenko<sup>1\*</sup>, O. Shtanko<sup>1</sup>, I. Sotnyk<sup>1</sup>, O. V. Prokopenko<sup>1</sup>

*1) Taras Shevchenko National University of Kyiv, Ukraine*

\* v.o.prokopenko AT gmail.com

Spin-torque microwave detectors (STMDs), which are based on ferromagnetic magnetic tunnel junctions (MTJs), are now considered as promising microwave signal detectors for a wide range of modern scientific and technological applications [1-4]. These detectors can have ultra-high volt-watt sensitivity, which greatly exceeds that of state-of-the-art Schottky diodes; they can also provide a very low minimum detectable microwave power and a high signal-to-noise ratio [1-3]. However, these positive features of STMDs have only been observed experimentally and explained theoretically and numerically for a single input harmonic microwave signal [1-3] or a small set of harmonic signals [4]. Conversely, the response of STMDs to non-harmonic signals, such as pulse signals, has been poorly analyzed, even though these pulse signals can naturally carry information and energy for conventional and unconventional digital computing and telecommunications devices, particularly neuromorphic spintronic devices. Therefore, the aim of this study is to analyze the response of an STMD to input microwave pulse signals, specifically the detector's output DC voltage  $U_{DC}$ .

We developed a numerical model of the magnetization dynamics, in an STMD under the action of an arbitrary, non-harmonic input microwave signal, which is characterized by the signal current  $I(t)$ . This model is based on the Landau-Lifshitz-Gilbert-Slonczewski equation for the unit magnetization vector,  $\mathbf{m}(t)$ , which includes the Berger-Slonczewski term that depends on  $I(t)$ . Using the numerically calculated  $\mathbf{m}(t)$  for a given  $I(t)$ , we calculate the magnetoresistance of the device  $R(t)$ . Next, we estimate the time-dependent output voltage of the detector,  $U(t) = I(t)R(t)$ , and finally calculate the time-averaged output DC voltage of the STMD  $U_{DC}$ .

We consider positive and symmetric rectangular pulses described by the signal current  $I(t)$ , with different pulse amplitudes ( $I_0 > 0$ ), durations ( $\tau$ ) and repetition periods ( $T$ ). As expected, the detector's response to pulse signals depends on the pulse type (positive or symmetric); however, the detector's behavior for both considered types of pulses is generally similar. At rather small pulse amplitudes,  $I_0 < I_{th}$ , the rectified voltage generated by an STMD depends linearly on  $I_0$  and the  $\tau/T$  ratio,  $U_{DC} \sim I_0(\tau/T)$ , corresponding to the linear regime of detector operation ( $I_{th}$  is the critical pulse amplitude). In this regime, some pulse characteristics (e.g., pulse amplitude  $I_0$  or the  $\tau/T$  ratio) can be unambiguously determined from the measured  $U_{DC}$  if the other pulse characteristics are known. In the other regime, which is observed when  $I_0 > I_{th}$ , the dependence of  $U_{DC}$  on  $I_0$  and  $\tau/T$  is nonlinear and nonmonotonic due to the strongly nonlinear magnetization dynamics, which prevent the unambiguous detection of the input pulse characteristics.

The obtained results can be important for the development of spintronic devices that detect and process pulse signals.

---

**KEYWORDS:** Spin-torque microwave detector, Pulse signal, Magnetization dynamics, Rectified voltage

---

**ACKNOWLEDGEMENTS:** This work was supported in part by grant No. 2025.07/0237 from the National Research Foundation of Ukraine. The authors thank all brave defenders of Ukraine who made it possible to finalize this publication.

### REFERENCES

- [1] G. Finocchio, R. Tomasello, B. Fang, A. Giordano, V. Puliafito, M. Carpentieri, and Z. Zeng, "Perspectives on spintronic diodes," *Appl. Phys. Lett.*, vol. 118, no. 16, p. 160502, April 2021.
- [2] R. Sharma, T. Ngo, E. Raimondo, A. Giordano, J. Igarashi, B. Jinnai, S. Zhao, J. Lei, Y.-X. Guo, G. Finocchio, S. Fukami, H. Ohno and H. Yang, "Nanoscale spin rectifiers for harvesting ambient radiofrequency energy," *Nat. Electron.*, vol. 7, no. 8, pp. 653-661, August 2024.
- [3] B. Fang, M. Carpentieri, S. Louis, V. Tiberkevich, A. Slavin, I.N. Krivorotov, R. Tomasello, A. Giordano, H. Jiang, J. Cai, Y. Fan, Z. Zhang, B. Zhang, J.A. Katine, K.L. Wang, P. Khalili Amiri, G. Finocchio, and Z. Zeng, "Experimental demonstration of spintronic broadband microwave detectors and their capability for powering nanodevices," *Phys. Rev. Appl.*, vol. 11, no. 1, p. 014022, January 2019.
- [4] D. Berkov, E.K. Semenova, "Numerical studies of the fundamental efficiency limit of a resonant in-plane spin-torque diode," *Phys. Rev. Appl.*, vol. 22, no. 4, p. 044040, October 2024.

## Spin-torque microwave detector with uniaxial magnetic anisotropy of the free magnetic layer

I. Fantych<sup>1\*</sup>, O. V. Prokopenko<sup>2</sup>

1) Institute of High Technologies Taras Shevchenko National University of Kyiv, Ukraine

2) Taras Shevchenko National University of Kyiv, Ukraine

\* lighspark AT gmail.com

Spin-torque microwave detectors (STMDs) are nanoscale spintronic devices based on magnetic tunnel junctions that generate an output DC (or low-frequency) voltage U<sub>DC</sub> when an input harmonic microwave signal current  $I(t)$  is applied [1-3]. In an STMD, the input signal current,  $I(t) = I_{AC} \sin(2\pi ft)$ , excites magnetization dynamics in the free magnetic layer (FL) of the detector, giving rise to AC variations of the device magnetoresistance  $R(t)$ . The mixing between the current  $I(t)$  and the magnetoresistance  $R(t)$  oscillations produces an output DC voltage  $U_{DC}$  if the frequency of magnetoresistance oscillations coincides with the input signal frequency  $f$  [1].

STMDs can have substantially better working characteristics than semiconductor detectors (e.g., Schottky diodes), however, these advantages are only available for certain operational regimes of STMDs that depend on the bias DC magnetic field, the magnetic anisotropy of the FL, the magnitude  $I_{AC}$  of the AC signal current [1, 3]. In particular, recently has been a growing interest in studying and applying STMDs with FLs made of anisotropic ferromagnetic materials [1, 3], such as L<sub>10</sub> materials, which are characterized by uniaxial magnetic anisotropy (UMA). The aim of this paper is to theoretically and numerically analyze the performance of an STMD with a FL that exhibits UMA.

Our analytic model is based on the Landau-Lifshitz-Gilbert-Slonczewski equation, which is written in the macrospin approximation for the unit magnetization vector  $\mathbf{m}(t)$ . The effective magnetic field in the equation includes contributions from the bias DC magnetic field, the demagnetization field, and the UMA field. Using spherical coordinates for  $\mathbf{m}(t)$ , we derive equations for the polar ( $\theta$ ) and azimuthal ( $\varphi$ ) angles of the vector  $\mathbf{m}(t)$ . By averaging these equations over the period of input signal oscillations,  $1/f$ , we can estimate the threshold current  $I_{th}$  required to excite sustainable magnetization dynamics, as well as the detector's output DC voltage  $U_{DC}$ .

Using the obtained analytical expressions, we calculate the dependence of the  $U_{DC}$  on the amplitude ( $I_{AC}$ ) and frequency ( $f$ ) of the input harmonic signal  $I(t)$  for different values of the UMA fields. We also estimate the power conversion ratio,  $P_{DC}/P_{AC}$ , as a function of these parameters. This ratio is defined as the output DC power of the detector ( $P_{DC}$ ) divided by the input AC power ( $P_{AC}$ ), and it characterizes the device's energy harvesting capability.

We found that in the out-of-plane magnetization precession regime, the UMA field defines the stable magnetization precession trajectory. The detector's output DC voltage  $U_{DC}$  and the  $P_{DC}/P_{AC}$  ratio moderately depend on the FL's UMA field. Additionally, using higher UMA fields can expand the detector's operating frequency band, and its power conversion ratio can reach  $\sim 10\%$ . We believe these results are important for the development and optimization of STMDs and STMD-based energy harvesters.

---

**KEYWORDS:** Spin-torque microwave detector, Uniaxial magnetic anisotropy, Magnetization dynamics, Rectified voltage, Energy harvesting

---

**ACKNOWLEDGEMENTS:** This work was supported in part by grant No. 2025.07/0237 from the National Research Foundation of Ukraine. The authors thank all brave defenders of Ukraine who made it possible to finalize this publication.

---

### REFERENCES

- [1] G. Finocchio, R. Tomasello, B. Fang, A. Giordano, V. Puliafito, M. Carpentieri, and Z. Zeng, “Perspectives on spintronic diodes,” *Appl. Phys. Lett.*, vol. 118, no. 16, p. 160502, April 2021.
- [2] K. Zeissler, “A compact spin-torque microwave detector,” *Nat. Electron.*, vol. 9, p. 340, April 2026.
- [3] B. Fang, M. Carpentieri, S. Louis, V. Tiberkevich, A. Slavin, I.N. Krivorotov, R. Tomasello, A. Giordano, H. Jiang, J. Cai, Y. Fan, Z. Zhang, B. Zhang, J.A. Katine, K.L. Wang, P. Khalili Amiri, G. Finocchio, and Z. Zeng, “Experimental demonstration of spintronic broadband microwave detectors and their capability for powering nanodevices,” *Phys. Rev. Appl.*, vol. 11, no. 1, p. 014022, January 2019.

## Possible microwave power redistribution due to the formation of magnon-plasmon-polaritons

O. V. Malyshev<sup>1\*</sup>, V. Y. Malyshev<sup>1</sup>, O. V. Prokopenko<sup>2</sup>, G. A. Melkov<sup>1</sup>

1) Institute of High Technologies Taras Shevchenko National University of Kyiv, Ukraine

2) Taras Shevchenko National University of Kyiv, Ukraine

\* oleksii.malyshev AT knu.ua

Surface electromagnetic waves (SEWs), which are often considered plasmon-polaritons (PPs), are coupled electromagnetic and electron density excitations [1, 2]. SEWs and PPs propagate along this interface between two media and their energy is localized near this interface, making them highly suitable for applications in modern surface physics and advanced electronics. These waves (quasiparticles) have been widely studied in the terahertz, infrared, and optical bands due to their strong field confinement, high sensitivity to material properties, and significant potential for developing various devices [1, 2]. However, the properties of SEWs and PPs in the microwave range, especially at the interface of magnetic conductors where magnon-plasmon-polaritons (MPPs) can be excited under certain conditions, are still poorly understood. Therefore, this paper aims to experimentally study the MPP formation process, which we believe is accompanied by microwave power redistribution.

We carried out our experiment in the Ka-band using a ferromagnetic surface electromagnetic wave resonator (FSEWR), which was a rectangular metal conducting film situated in a below-cutoff waveguide [3]. The incident electromagnetic wave excites PPs in the FSEWR. When a certain in-plane DC bias field is then applied to the resonator, the electromagnetic field of the incident wave also excites magnetization oscillations (magnons) in the FSEWR, which can force the formation of MPPs. This process requires additional energy, the binding energy of magnons and PPs, which can be measured experimentally.

In our experiment, we precisely measured the microwave power incident on, reflected from, and transmitted through the FSEWR, and calculated the power losses in the FSEWR. Our experimental results demonstrate that losses increase up to four times when the bias DC magnetic field of ~500 mT required for magnon excitation is applied. At the same time, the resonator frequency changes by ~0.5% (0.13 GHz), and the reflection coefficient at resonance changes by approximately three times. We believe these results can be explained by the redistribution of microwave power due to MPP formation.

The obtained results are important for the physics and applications of microwave MPPs and for the development of magnetic film-based microwave plasmonic devices that can be tuned by DC magnetic fields.

---

**KEYWORDS:** Surface plasmon, Plasmon polariton, Microwave resonator, Ferromagnet, Film

---

**ACKNOWLEDGEMENTS:** The work was carried out with funding from the Ministry of Education and Science within the framework of international scientific and technical bilateral cooperation in accordance with the Protocol of the 11th meeting of the Ukrainian-Austrian Joint Commission on Scientific and Technical Cooperation in implementation of the Agreement on Scientific and Technical Cooperation between the Cabinet of Ministers of Ukraine and the Government of the Republic of Austria of June 6, 2003, signed on April 15, 2025 (M/68-2025). The authors would like to thank all the brave defenders of Ukraine who made the finalization of this publication possible.

---

### REFERENCES

- [1] M. Aftab, M. S. Mansha, T. Iqbal *et al.*, “Surface plasmon excitation: Theory, configurations, and applications”, *Plasmonics*, vol. 19, pp. 1701-1719, 2024.
- [2] R. Tong, R. Zhang, P. Yuan, S. Li, L. Liu, and Y. Zhao, “Tamm plasmon polaritons: Principle, excitation, and sensing applications”, *Laser & Photonics Reviews*, 2025, Art. no. e02507.
- [3] O.V. Malyshev, V.Yu. Malyshev, O.V. Prokopenko, “A New Method of Study of Microwave Magnon-Plasmon-Polaritons” in 2023 IEEE 13th International Conference Nanomaterials: Applications & Properties (NAP). IEEE, p. 07nmm-22, September 2023.

## Visualizing local phonons and edge state magnetism on 7-atom wide armchair graphene nanoribbons

S. Šćepanović<sup>1</sup>\*, J. Mirković<sup>1</sup>, A. Hassanien<sup>2</sup>

1) University of Montenegro, Montenegro

2) Jozef Stefan Institute, Slovenia

\* stefanscepanovic AT gmail.com

Graphene nanoribbons (GNRs) offer a suitable platform for carbon-based spintronics due to their negligible spin-orbit coupling, yet practical spin devices require precise control over magnetic moments, contacts, decoherence, and edge-state engineering. Here, we present a combined STM/STS/IETS study of 7-AGNRs on Au(111) addressing fundamental spin phenomena in such nanoscale systems. We demonstrate that controlled hydrogen abstraction at zigzag termini induces delocalized Kondo resonances extending  $\sim 2.5$  nm along the edges. Temperature-dependent spectroscopy reveals a Kondo temperature of  $\sim 68$  K [1], with DFT confirming weak inter-state coupling despite substrate screening, highlighting robust intrinsic edge magnetism. To optimize charge transport, we engineer C-Au covalent bonds that lift GNRs into suspended configurations, eliminating substrate quenching and revealing a pristine bandgap of 2.78 eV [2]. These suspended GNRs has been utilized as functionalized STM tips which enabling high-resolution imaging of edge-state quantum interference. This way we obtain enhanced inelastic tunneling spectroscopy maps of longitudinal and shear-like phonon modes localized at the armchair edges [3], which remain protected from substrate scattering. These edge-protected vibrations are critical for understanding spin-phonon coupling and coherence limits.

---

**KEYWORDS:** Graphene nanoribbons, Spin phenomena, Kondo effect, Spintronics, Inelastic tunneling spectroscopy

---

**ACKNOWLEDGEMENTS:** The authors acknowledge the financial support from the Ministry of Education, Science and Innovation of the Government of Montenegro under project 04-082123-252911 (NOQUMNANO), the Slovenian Research Agency (ARIS) under Program No. P1-0099, the European Cooperation in Science and Technology via COST Action CA21144 (SUPERQUMAP) and the Montenegrin Science Promotion Foundation for the work and participation in the 2026 IEEE 16th International Conference Nanomaterials: Applications & Properties.

---

### REFERENCES

- [1] Šćepanović, S., A. Kimouche, Mirković, J. *et al.* Delocalized spin states at zigzag termini of armchair graphene nanoribbon. *Sci Rep* 14, 11641 (2024). <https://doi.org/10.1038/s41598-024-62624-9>
- [2] A. Hassanien, Robust Contact by Direct Formation of C-Au Bond in Suspended Armchair Graphene Nanoribbon. *Phys. Status Solidi RRL*, 18: 2400192. (2024) <https://doi.org/10.1002/pssr.202400192>
- [3] Šćepanović, S., López-D. Alcalá, J.J. Baldoví, A. Vahl, Hassanien, A. *Phys. Status Solidi RRL*. (2025); 19:e2500203. <https://doi.org/10.1002/pssr.202500203>

## Spectroscopic ellipsometry evidence of Mn level hybridization in (Ga,Mn)(As,P)

N. Tataryn<sup>1\*</sup>, O. Yastrubchak<sup>1</sup>, S. Mamykin<sup>1</sup>, O. Kondratenko<sup>1</sup>, V. Romanyuk<sup>1</sup>, B. A. Assaf<sup>2</sup>, X. Liu<sup>2</sup>,  
J. Furdyna<sup>2</sup>

1) V.E. Lashkaryov Institute of Semiconductor Physics, National Academy of Sciences of Ukraine, pr. Nauky 41, 03028, Kyiv, Ukraine, Ukraine

2) Department of Physics and Astronomy, University of Notre Dame, Notre Dame, IN 46556 USA, USA

\* natalko1996 AT gmail.com

The dilute ferromagnetic semiconductors (DFSs) based on III-Mn-V alloys are prototypical systems for studying the interplay between spin and charge degrees of freedom in solids and have played a central role in the development of spin-based electronic concepts. In these materials, Mn simultaneously supplies localized magnetic moments and itinerant holes, leading to carrier-mediated ferromagnetism. As a consequence, tuning the electronic structure is intrinsically coupled to the magnetic dopant concentration, limiting independent control of exchange and band structure.

A key route to overcome this limitation is chemical alloying of the host lattice, which modifies band structure and impurity levels without directly altering Mn content. In particular, (Ga,Mn)(As,P) offers a unique platform in which the electronic structure can be tuned via the As/P ratio, in addition to Mn concentration and thermal processing. In this system, substitutional Mn at Ga sites acts as an acceptor, with its binding energy increasing significantly from  $\sim 0.11$  eV in (Ga,Mn)As to  $\sim 0.4$  eV in (Ga,Mn)P, suggesting a continuous tuning of the degree of p-d hybridization with increasing P content.

Despite extensive studies, the fundamental nature of Mn-derived electronic states in III-Mn-V ferromagnetic semiconductors remains unresolved: whether they form valence-band-hybridized states or more localized impurity-like states. This distinction is governed by the strength of hybridization between Mn 3d states and anion p states, which ultimately controls the character of the exchange interaction.

Here, we employ spectroscopic ellipsometry (SE) to probe the evolution of Mn-derived electronic states in (Ga,Mn)(As,P) as a function of phosphorus concentration and post-growth annealing.

The SE results provide a coherent picture of how phosphorus incorporation modifies the character of Mn levels in (Ga,Mn)(As,P). The nature of the Mn-induced acceptor state evolves as a function of its energetic separation from the valence-band maximum. When the acceptor level lies close to the valence-band edge, the Mn states retain a predominantly hybridized, valence-band-like character and remain partially delocalized over neighboring anion sites. As the valence-band edge shifts further away from the Mn levels with increasing P concentration, the Mn states acquire a progressively more Mn-centered character. This results in stronger localization on the Mn 3d orbitals and eventually leads to the formation of a separated impurity band. These strongly localized states give rise to pronounced atomic-like d-d transitions, which are clearly resolved in the SE spectra. Our SE measurements also demonstrate pinning of the Fermi level, making  $E_0$  virtually independent of P content. Nevertheless, we have clearly shown here that (Ga,Mn)(As,P) offers a versatile platform on which the fundamental aspects of impurity physics can be reliably tuned using chemical controls.

---

**KEYWORDS:** Dilute ferromagnetic semiconductors (DFSs), P-d hybridization, (Ga, P) alloys, Spectroscopic ellipsometry (SE)

---

**ACKNOWLEDGEMENTS:** B. A. A. and X. L. acknowledge support from National Science Foundation grant DMR-2313441. O. Y., V. R., O. K., and S. M. acknowledge the National Research Foundation of Ukraine for financial support of this research (Project number 2025.07/0271).

## Synchronization dynamics in a dual-antiferromagnetic-layer spin Hall oscillator

O. Shtanko<sup>1\*</sup>, O. V. Prokopenko<sup>1</sup>

1) Taras Shevchenko National University of Kyiv, Ukraine

\* olegshtanko2000 AT gmail.com

Antiferromagnetic (AFM) materials are promising for ultrafast spintronics due to their intrinsic terahertz-frequency dynamics, robustness against external magnetic-field perturbations, and nearly vanishing stray fields, which support stable high-density integration [1]. These properties can be exploited in an antiferromagnetic spin Hall oscillator (AFM SHO), typically realized as a Pt/AFM bilayer, where a DC charge current induces a spin current via the spin Hall effect and generates spin-transfer torque that drives self-sustained oscillations of the AFM sublattice magnetizations. However, conventional single-layer AFM SHOs remain limited by a narrow frequency-tuning range (0.1-2.0 THz) and output power below the  $\sim 1 \mu\text{W}$  technological benchmark [2,3]. Mutual synchronization of phase-locked oscillators can overcome these limitations by producing a stronger coherent collective output. This paper investigates the synchronization dynamics of a dual-antiferromagnetic-layer spin Hall oscillator (DAL SHO) within a vertical Pt/AFM/S/AFM/Pt heterostructure. Unlike spatially distributed arrays, this single device internally couples two identical, current-driven canted AFM layers via spacer-mediated magnetodipolar interaction. We model this system using coupled Landau-Lifshitz-Gilbert-Slonczewski equations to track the four sublattice magnetization vectors. The comprehensive effective field accounts for exchange, magnetic anisotropies, the Dzyaloshinskii-Moriya interaction, spin-pumping-enhanced damping, spin-transfer torque, and cross-demagnetization coupling. By varying the direct current density in one platinum layer, we effectively control the frequency detuning between the two interacting AFM subsystems. Analysis of the time-dependent Néel vectors confirms a stable phase-locked state characterized by zero relative frequency detuning and a constant phase offset of  $\sim 0.28$  rad. With a fixed bottom-layer current, magnetodipolar coupling merges the initially distinct frequencies, yielding a shared synchronization bandwidth of nearly 100 GHz (spanning 230-330 GHz for top currents of  $1.3\text{-}2.7 \cdot 10^8 \text{ A/cm}^2$ ). Notably, expanding the spacer thickness from 6 to 26 nm attenuates this cross-demagnetization coupling, systematically compressing the synchronization window from 110 GHz down to 80 GHz. The obtained results demonstrate that the DAL SHO can support internal synchronization driven by spacer-mediated magnetodipolar coupling. The synchronization dynamics can be controlled dynamically through the applied current and structurally through the spacer thickness. This makes the DAL SHO a promising compact platform for coherent upper-sub-terahertz signal generation, controllable phase locking, and future networks of synchronized antiferromagnetic spintronic oscillators.

**KEYWORDS:** Antiferromagnet, Spin Hall oscillator, Terahertz frequency, Mutual synchronization

**ACKNOWLEDGEMENTS:** This work was partially supported by the National Research Foundation of Ukraine under grant No. 2025.07/0237. The authors express their sincere gratitude to all the brave defenders of Ukraine, whose courage and sacrifice made the completion of this publication possible.

### REFERENCES

- [1] Z. Guo, X. Wang, W. Wang, G. Zhang, X. Zhou, and Z. Cheng, “Spin-polarized antiferromagnets for spintronics,” *Adv. Mater.*, vol. 37, no. 36, Art. no. 2505779, Jun. 2025.
- [2] R. Khymyn, I. Lisenkov, V. Tiberkevich, B. A. Ivanov, and A. Slavin, “Antiferromagnetic THz-frequency josephson-like oscillator driven by spin current,” *Sci. Rep.*, vol. 7, no. 1, p. 43705, Mar. 2017.
- [3] O. R. Sulymenko, O. V. Prokopenko, V. S. Tiberkevich, A. N. Slavin, B. A. Ivanov, and R. S. Khymyn. “Terahertz-frequency spin Hall auto-oscillator based on a canted antiferromagnet,” *Phys. Rev. Appl.*, vol. 8, no. 6 p. 064007, December 2017.

# Track 8

Superconductivity in Nanoscale and Mesoscopic Systems

## Magnetic landscape of superconducting resonators under radio-frequency excitation

J. Baumgarten<sup>1</sup>, N. Lejeune<sup>1</sup>, L. Nulens<sup>2</sup>, I. P. Cools<sup>3</sup>, J. Van de Vondel<sup>2</sup>, A. Silhanek<sup>1\*</sup>

1) *Université de Liège, Belgium*

2) *KU Leuven, Belgium*

3) *Chalmers University of Technology, Sweden*

\* asilhanek AT uliege.be

Superconducting resonators are essential components in quantum circuits and highly sensitive sensors. However, their performance is often compromised by magnetic flux penetration, as the interaction of flux quanta and the induced radio-frequency (RF) currents in the superconducting thin film leads to significant energy dissipation. At low operating temperatures, this issue is aggravated as thermomagnetic instabilities can trigger the sudden propagation of magnetic flux avalanches. An important open question is whether the RF excitation itself stimulates the nucleation and propagation of magnetic flux avalanches in the superconducting thin film. The literature remains inconclusive on this point, partly due to the lack of compelling evidence for this phenomenon. In this presentation, we address this challenge by directly visualizing magnetic flux penetration through Faraday rotation imaging under simultaneous RF excitation [1]. We demonstrate that the avalanche activity exhibits a weak dependence on the RF intensity. However, magnetic flux bursts clearly influence the RF transmission properties of the device. Furthermore, we can unambiguously associate a particular avalanche event with a jump in resonance frequency. This enables us to identify the loci of most deleterious events and understand the distinct origins of upward and downward frequency shifts. These observations are supported by electromagnetic simulations in which local changes of the kinetic inductance mimic flux avalanches and confirm the invasive character of the MOI technique. The insights gained from this study aim to contribute to the broader understanding of the magnetic resilience of superconducting resonators and to improve their efficiency and stability.

---

**KEYWORDS:** Superconducting resonators, Magneto-optical imaging, Magnetic flux avalanches, Vortex dynamics

---

**ACKNOWLEDGEMENTS:** The authors acknowledge financial support from Fonds de la Recherche Scientifique - FNRS under the grant Weave PDR T.0208.23, and the Research Foundation and by COST (European Cooperation in Science and Technology) [www.cost.eu] through COST Action SUPERQUMAP (CA 21144). N. L. acknowledges support from FRS-FNRS (Research Fellowships FRIA).

---

### REFERENCES

- [1] J. Baumgarten, N. Lejeune, L. Nulens, I. P. C. Cools, J. Van de Vondel, and A. V. Silhanek, Magnetic landscape of NbTiN superconducting resonators under radio-frequency excitation; <https://doi.org/10.48550/arXiv.2603.08500>

## DC-operated Josephson junction arrays as a cryogenic on-chip microwave measurement platform

J. Van de Vondel<sup>1\*</sup>, S. Vervoort<sup>1</sup>, L. Nulens<sup>1</sup>, D. Chaves<sup>2</sup>, H. Dausy<sup>1</sup>, S. Reniers<sup>1</sup>, M. Abouelela<sup>3</sup>, I. P. Cools<sup>4</sup>, A. Silhanek<sup>5</sup>, M. Van Bael<sup>1</sup>, B. Raes<sup>6</sup>

1) KU Leuven, Belgium

2) Brazilian Center for Research in Physics, Brazil

3) TU Delft, Netherlands

4) Chalmers University of Technology, Sweden

5) Université de Liège, Belgium

6) IMEC, Belgium

\* joris.vandevondel AT kuleuven.be

The control and readout of superconducting qubits conventionally relies on signals within the 4-8 GHz frequency range [1]. However, existing systems face challenges, as the high-frequency signal is typically generated at room temperature and transmitted through multiple attenuation stages to the cryogenic environment, inducing noise and lacking scalability [2]. Addressing these issues, it is more beneficial to situate the control circuits near the qubit devices.

As a step towards this goal, we leverage arrays of weak link Josephson junctions as on-chip signal generators capable of converting DC voltage into AC current, emitting voltage-tunable radiation according to the Josephson relations [3]. We successfully fabricated such arrays, utilizing superconducting MoGe and NbTiN islands with dimensions of  $500 \times 500$  nm<sup>2</sup>, placed on a 5 nm-thick Au film as the weak link material [4]. The detected RF signal emitted by the arrays when biased with a DC voltage shows high-power regions consistent with the Josephson relation, confirming coherent emission. The emitted radiation can be further tuned using temperature, magnetic fields, applied currents, and device design. Furthermore, a clone of the SNS junction arrays can also serve as a fully DC-operated microwave radiation detector, leading us to propose a high-frequency measurement platform entirely based on DC instrumentation and wiring.

---

**KEYWORDS:** Superconducting devices, Josephson junctions, Cryogenic microwave sources

---

**ACKNOWLEDGEMENTS:** This work is supported by Research Foundation Flanders (FWO) grant number 11K6525N and 11A3V25N, and under the grant Weave G0D7723N, the EUCOST action SUPERQUMAP CA21144, the Fonds de la Recherche Scientifique - FNRS under the grant Weave -PDR T.0208.23 and CDR J.0199.25. This research is supported and funded by an interuniversity BOF project (IBOF-23-065).

---

### REFERENCES

- [1] P. Krantz, *et al.*, Appl. Phys. Rev. 6, 021318 (2019)
- [2] A. Potočník, Nature Electronics volume 8, 3 (2025)
- [3] B.D. Josephson, Phys. Lett. 1, 251 (1962)
- [4] S. Vervoort *et al.*, Commun. Phys. 8, 292 (2025)

## Spin mixing in Ising superconductors

P. Jureczko<sup>1</sup>, J. Haniš<sup>2</sup>, P. E. D. F. Junior<sup>3</sup>, M. Gmitra<sup>2, 4</sup>, M. Kurpas<sup>1 \*</sup>

1) Institute of Physics, University of Silesia in Katowice, Poland

2) Institute of Physics, Pavol Jozef Šafárik University in Košice, Slovakia

3) University of Central Florida, USA

4) Centre of Low Temperature Physics, Institute of Experimental Physics, Slovak Academy of Sciences, Slovakia

\* marcin.kurpas AT us.edu.pl

The immunity of Ising superconductors to external magnetic fields originates from a spin locking of the paired electrons to an intrinsic Zeeman-like field [1]. In non-centrosymmetric crystals, spin-momentum locking generates type-I Ising pairing, where the direction of the intrinsic field can be inferred directly from the spin expectation values. In contrast, centrosymmetric materials host type-II Ising pairing: here, electron spins locked to orbital degrees of freedom form Cooper pairs from spin-orbit-split doublets [2]. Time-reversal symmetry enforces spin degeneracy within each doublet, obscuring the spin polarization of the bands and complicating the determination of the spin-orbit field direction.

We introduce an efficient framework for identifying Ising pairing based on the spin-mixing parameter  $b^2$  [6]. To validate this approach, we perform first-principles calculations for monolayer transition-metal dichalcogenide superconductors PdTe<sub>2</sub>, NbTe<sub>2</sub>, and TiSe<sub>2</sub>. We compute  $b^2$  for individual Fermi pockets and construct a comprehensive picture of possible type-II Ising pairing throughout the Brillouin zone. Complementing these results, we use group-theoretical analysis to elucidate the structure of spin-orbit coupling and the microscopic origin of spin mixing in the bands forming the Fermi surfaces.

Our analysis shows that, contrary to expectations based solely on spin-orbit locking, not every spin-orbit-split doublet contributes to Ising pairing. Finally, by relating the spin-mixing parameter  $b^2$  to the intrinsic out-of-plane Zeeman field, we estimate the corresponding upper critical in-plane magnetic field. The proposed framework can be readily implemented in commonly used density-functional-theory packages and tight-binding approaches, providing an efficient tool for screening candidate type-II Ising superconductors.

---

**KEYWORDS:** Ising superconductivity, First principles calculations, Spin mixing

---

### REFERENCES

- [1] J. M. Lu, O. Zheliuk, I. Leermakers, N. F. Q. Yuan, U. Zeitler, K. T. Law, J. T. Ye, Evidence for two-dimensional Ising superconductivity in gated MoS<sub>2</sub> Science 350, 1353 (2015)
- [2] M. Liao, Y. Zang, Z. Guan, H. Li, Y. Gong, K. Zhu, X.-P. Hu, D. Zhang, Y. Xu, Y.-Y. Wang, K. He, X.-C. Ma, S.-C. Zhang, Q.-K. Xue, Superconductivity in Few-Layer Stanene, Nat. Phys. 14, 344 (2018)
- [3] P. Jureczko, J. Haniš, P. E. Faria Junior, M. Gmitra, and M. Kurpas, Probing type-II Ising pairing using the spin-mixing parameter, Phys. Rev. B 109, 165428 (2024)

## Recent progress of NbN-based superconducting quantum bits

T. Yamashita<sup>1</sup>\*

1) Tohoku University, Japan

\* taro AT tohoku.ac.jp

Development of superconducting quantum computers has been actively pursued worldwide in recent years. In this talk, we will present our recent progress of various types of high-coherence superconducting quantum bits (qubits) with niobium nitride (NbN)-based Josephson junctions.

First one is NbN-based transmon with the sidewall spacer (SWS) structure. We fabricated NbN/AlN/NbN junctions with this structure in which the lossy insulating layer (SiO<sub>2</sub>) exists only near the junction sidewalls. In the sidewall spacer structure, the volume of SiO<sub>2</sub> is much less than that in the conventional structure, making it easier to remove SiO<sub>2</sub> using buffered hydrogen fluoride at the end of the process. We developed sidewall spacer-passivated junctions with varying the AlN thicknesses and measured their current-voltage characteristics at 10 mK and 2.2 K. As a result, we observed that the high subgap resistance and the low critical current density ( $J_c$ ) of 15.8 A/cm<sup>2</sup>, which were suitable for the qubits. Furthermore, we achieved reliable control of  $J_c$  with excellent characteristics over a wide range of the AlN thickness. By using this technique, we developed transmons with SWS structure and achieved the excellent lifetime over 100  $\mu$ s which is significant improvement as non-Al-based qubits.

Second topic is self-shunted flux qubits (SSFQs) [1]. Among the various types of superconducting qubits, a flux qubit with three Josephson junctions which shows the high anharmonicity is a promising candidate for the large-scale superconducting quantum computer. However, the shunt capacitor in the flux qubits drastically increases the device footprint and becomes a bottleneck for large-scale integration. To achieve both the large anharmonicity and small footprint, we propose and demonstrate a ultracompact SSFQs in which the shunt capacitance is provided by the large-area Josephson junctions [1]. We observed the large anharmonicity of 790 MHz as well as the long lifetime of 24.7  $\mu$ s, which is the longest value reported for flux qubits without the shunt capacitors.

Another issue of the scalability of the flux qubit was the need of the half-flux-quantum bias to achieve the flux-insensitive point (longest coherence time). Theoretically, it has been presented that the flux-bias-free operation could be achieved by incorporating the ferromagnetic Josephson junction ( $\pi$ -junction) in the qubits [2]. In this work, as a novel Josephson junction technique to realize the flux-bias-free flux qubits, we developed the NbN-based ferromagnetic  $\pi$ -junctions with a diluted ferromagnetic interlayer of CuNi or PdNi and their  $\pi$ -shift [3-5]. In recent years, we have successfully confirmed the flux-bias-free operation of the flux qubits with the NbN-based  $\pi$ -junction in the microwave cavity [5]. The demonstrated flux-bias-free qubit showed the reasonable coherence time of 1.5  $\mu$ s, which was three orders of magnitude higher than that of the previously reported phase qubit with the  $\pi$ -junction.

---

**KEYWORDS:** Superconducting qubit, Josephson junction,  $\pi$ -junction, Nitride

---

**ACKNOWLEDGEMENTS:** This work was partly supported by JSPS KAKENHI (25H00406, JP19H05615), JST CREST (JPMJCR24I5, JPMJCR1775), and JST Moonshot R&D Program (JPMJMS2067). TY acknowledges Center for Heterogeneous Quantum/Material Fusion Technologies, Center for Key Interdisciplinary Research, Tohoku University.

---

### REFERENCES

- [1] T. Uchida, H. Kutsuma, T. Yamashita., “Self-Shunted Superconducting Flux Qubit”, IEEE Transactions on Applied Superconductivity 34, 1 (2024).
- [2] T. Yamashita, K. Tanikawa, S. Takahashi, S. Maekawa, “Superconducting Qubit with a Ferromagnetic Josephson Junction”, Physical Review Letters 95, 097001 (2005).
- [3] T. Yamashita, A. Kawakami, H. Terai., “NbN-Based Ferromagnetic 0 and  $\pi$  Josephson Junctions”, Physical Review Applied 8, 054028 (2017).
- [4] D. Pham, R. Sugimoto, K. Oba, Y. Takeshita, F. Li, M. Tanaka, T. Yamashita, A. Fujimaki, “Weak spin-flip scattering in Pd<sub>89</sub>Ni<sub>11</sub> interlayer of NbN-based ferromagnetic Josephson junctions”, Scientific Reports 12, 6863 (2022).
- [5] S. Kim, L.V. Abdurakhimov, D. Pham, W. Qiu, H. Terai, S. Ashhab, S. Saito, T. Yamashita, K. Semba, “Superconducting flux qubit with ferromagnetic Josephson  $\pi$  junction operating at zero magnetic field”, Communications Materials 5, Article number: 216 (2024).

## Engineering electronic phase transitions in cuprate superconductors: From nanoscale oxygen control to cryogenic memory

A. Palau<sup>1</sup>\*

*1) Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain*

\* palau AT icmab.es

High-temperature cuprate superconductors exhibit an exceptionally rich phase diagram in which superconductivity, correlated metallic states, and insulating phases are significantly affected by oxygen stoichiometry and carrier density. Effectively controlling this sensitivity in a scalable and precise manner is crucial for both fundamental research and the development of superconducting devices. In this study, we present an integrated experimental approach to engineer and exploit electronic phase transitions in epitaxial  $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$  (YBCO) thin films through local direct laser writing and electric-field modulation of oxygen content and hole concentration. Initially, we demonstrate nanoscale spatial tuning of superconductivity via maskless direct laser writing under ambient conditions. By locally inducing controlled oxygen depletion, sub-micrometer grayscale patterns are created over large areas, enabling continuous and reversible modulation of the superconducting critical temperature, carrier density, and critical current density. Cryogenic magneto-optical imaging directly visualizes the spatial redistribution of superconductivity and magnetic flux penetration, while transport measurements confirm systematic tuning of both normal-state and superconducting properties. Correlated Raman spectroscopy and optical reflectometry identify laser-power-dependent oxygen depletion without structural damage, establishing direct laser writing as a non-destructive, scalable method to navigate the cuprate phase diagram and engineer superconducting nanostructures with locally programmed functionality [1]. Building on controlled oxygen landscapes, we further explore electric-field-induced metal-insulator transitions in YBCO-based heterostructures for cryogenic memory applications. These devices exhibit non-volatile, multilevel resistive switching that persists well below the superconducting transition temperature. Two competing mechanisms are identified: electrochemical oxygen vacancy migration dominant at high temperatures, and a low-temperature electrostatic transition driven by hole redistribution within an oxygen-depleted interfacial layer. The latter enables low-voltage, highly stable analog resistance states and reproducible potentiation-depression cycles. A physics-based compact model accurately reproduces the experimental behavior and supports circuit-level simulations for cryogenic in-memory and neuromorphic computing architectures [2]. Finally, complementary magnetotransport measurements reveal anomalous in-plane magnetoresistance and planar Hall effects near the superconducting transition, indicating unconventional quasiparticle transport and a previously underappreciated spin-orbit landscape in cuprate superconductors.

**KEYWORDS:** High-temperature cuprate superconductors, Field-induced carrier doping, Direct laser writing, Metal-insulator transition, Cryogenic memory applications

**ACKNOWLEDGEMENTS:** Spanish Ministry of Science and Innovation, MCIN/ AEI /10.13039/501100011033/ through the “Severo Ochoa” Programme CEX2023-001263-S, HTSUPERFUN PID2021-124680OB-I00, HTS-4ICT PID2024-156025OB-I00, co-financed by ERDF A way of making Europe. The Spanish Nanolito networking project (RED2022-134096-T). The European COST Action SUPERQUMAP (CA 21144). AGAUR (2022 FISDU 00115).

### REFERENCES

- [1] I. Biancardi, V. Levati, J. Alcalà, T. Günkel, N. Lejeune, A.V. Silhanek, V. Russo, N. Mestres, D. Petti, A. Palau, E. Albisetti “Nanoscale Spatial Tuning of Superconductivity in Cuprate Thin Films via Direct Laser Writing”, arXiv:2601.09513 (2026)
- [2] T Günkel, J. Alcalà, A. Fernández, A. Barrera, Ll. Balcells, N. Mestres, E. Miranda, J. Suñé, A. Palau. “Field-Induced Phase Transitions in Cuprate Superconductors for Cryogenic in-Memory Computing” *Small*, 2411908 (2025)

## Reactive sputtering optimization of ultrathin NbTiN films for superconducting nanowire single photon detector applications

T. Ščepka<sup>1\*</sup>, J. Šoltýs<sup>1</sup>, I. Vetrova<sup>2</sup>, M. Precner<sup>1</sup>, Z. Zápražný<sup>2</sup>, I. Piš<sup>1</sup>, P. Neilinger<sup>3</sup>, M. Baránek<sup>3</sup>, S. Kern<sup>3</sup>, M. Grajcar<sup>3</sup>

1) Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava, Slovakia

2) Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská cesta 9, 84104 Bratislava, Slovakia

3) Department of Experimental Physics, Faculty of Mathematics, Physics and Informatics, Comenius University Bratislava, Slovakia

\* tomas.sceпка AT savba.sk

Ultrathin niobium titanium nitride (NbTiN) films are widely used in superconducting nanowire single-photon detectors (SNSPDs) due to their high critical temperature, fast response, and compatibility with nanofabrication processes [1-3]. In this work, NbTiN thin films with thicknesses ranging from 3 to 12 nm were deposited on sapphire substrates by reactive magnetron sputtering using dual-target Nb (DC) and Ti (RF) sources. The influence of substrate temperature and nitrogen content in the sputtering atmosphere on the structural, electrical, and superconducting properties of the films was systematically investigated. The films were deposited at substrate temperatures ranging from room temperature to 600 °C under varying Ar/N<sub>2</sub> gas ratios, while maintaining a working pressure of 3 mTorr. Sheet resistance measurements, superconducting transition characterization, and X-ray photoelectron spectroscopy were used to evaluate transport properties, stoichiometry, and disorder effects. Additional thickness-dependent measurements were performed to assess the evolution of superconductivity in ultrathin films. A clear correlation between deposition temperature and superconducting performance was observed. Increasing substrate temperature reduced sheet resistance and enhanced the critical temperature, indicating improved crystallinity, reduced disorder, and optimized nitrogen incorporation. Notably, NbTiN films deposited under nitrogen-rich conditions demonstrated robust superconductivity despite operation in a strongly poisoned sputtering regime. For a 7 nm film deposited at 600°C under an Ar/N<sub>2</sub> flow ratio of 50/50 sccm, a sheet resistance of approximately 300 fi/sq was obtained, corresponding to a resistivity of about 210 μfi·cm, suggesting a dense and moderately disordered superconducting state. All films with thicknesses greater than 5 nm, deposited at 600°C, showed critical temperatures above 10 K. The obtained results indicate that optimized NbTiN films for SNSPD applications require a balance between superconducting strength and controlled disorder. The combination of moderate sheet resistance and elevated critical temperature suggests that high-temperature reactive sputtering can stabilize high-quality NbTiN even under high nitrogen fractions. These findings provide insight into process-structure-property relationships in ultrathin superconducting nitrides and support the development of reproducible SNSPD-grade NbTiN thin films.

**KEYWORDS:** NbTiN thin films, Reactive sputtering, Superconducting nanowire single-photon detectors, Ultrathin films, Disorder engineering

**ACKNOWLEDGEMENTS:** This work is supported by the VEGA agency, grant number VEGA-2/0167/26.

### REFERENCES

- [1] S. Dong, D.M.Z. Koh, F. Martinelli, P.J.E. Brosseau, M. Petrovic, L. Shen, G. Adamo, A.N. Vetlugin, Sidorova. M., Kurtsiefer, Ch., C. Soci, Establishing an end-to-end workflow for SNSPD fabrication and characterization. *Sci Rep* 14, 30891, (2024).
- [2] J. Zichi, J. Chang, S. Steinhauer, K. Von Fieandt, J.W. Los, G. Visser, N. Kalhor, T. Lettner, A.W. Elshaari, I.E. Zadeh, V. Zwiller, Optimizing the stoichiometry of ultrathin NbTiN films for high-performance superconducting nanowire single-photon detectors. *Optics express*, 27(19), (2019).
- [3] X. Yang, L. You, L. Zhang, C. Lv, H. Li, X. Liu, H. Zhou, Z. Wang, Comparison of superconducting nanowire single-photon detectors made of NbTiN and NbN thin films. *IEEE Transactions on Applied Superconductivity*, 28(1), (2017).

## Features of phonon spectrum degeneracies at the R point of A15-type crystals

D. Kaynts<sup>1</sup>\*, I. Nebola<sup>2</sup>, A. Korneichuk<sup>3</sup>, R. Zosimov<sup>2</sup>, O. Maksakova<sup>4</sup>

1) Uzhhorod National University, Uzhhorod, Ukraine

2) Uzhhorod National University, Ukraine

3) Uzhgorod National University, Ukraine

4) Education and Research Institute “School of Physics and Technology”, V.N. Karazin Kharkiv National University, Ukraine

\* diana.kaynts AT uzhnu.edu.ua

Phonon spectra play a central role in understanding the dynamical stability and lattice properties of intermetallic compounds. In particular, A<sub>15</sub>-type materials exhibit unusual structural and vibrational characteristics, for example, superconductivity, that make them a long-standing subject of condensed matter research.

A<sub>15</sub> compounds such as Mo<sub>3</sub>X and Cr<sub>3</sub>X (X = Ge, Si) are characterized by a complex cubic structure (space group Pm-3n) with strong symmetry constraints. These features lead to highly structured phonon dispersions and enable symmetry-driven degeneracies at high-symmetry points of the Brillouin zone. However, the origin and robustness of phonon degeneracies in A<sub>15</sub> systems, particularly at the R point, remain not fully clarified.

In this work, a symmetry-consistent lattice-dynamical framework is developed using a superlattice representation of the A<sub>15</sub> structure. The crystal is described within a (4a × 4a × 4a) simple cubic metric, resulting in a complete model with 64 effective lattice positions. A dual description in terms of lattice nodes and modulation vectors is introduced, allowing the dynamical problem to be formulated in a modal basis.

Here we show that the phonon spectrum at the R point exhibits a characteristic set of symmetry-protected degeneracies that remain robust under variation of model parameters. The obtained structure arises from symmetry constraints of lattice dynamics rather than from accidental parameter tuning. Compared to simplified approaches, the results reveal a stable degeneracy pattern with high-multiplicity states, indicating that such features are intrinsic to the A<sub>15</sub> family as shown in [1-5].

These findings provide additional insight into the role of symmetry in determining vibrational properties of complex intermetallic systems and may be relevant for materials with strong lattice-coupling effects. Overall, symmetry-protected phonon degeneracies can be regarded as a characteristic fingerprint of the A<sub>15</sub> structural class.

---

**KEYWORDS:** Superlattice, Phonon spectra, Modulation vector, Superconductors, Phonon degeneracy

---

### REFERENCES

- [1] F. Weiss, O. Demolliens, R. Madar, J.P. Senateur, R. Fruchart. On the stabilization of A-15 Nb<sub>3</sub>Ge with high TC's. *Journal de Physique*, 45 (7), pp.1137-1141. (10.1051/jphys:019840045070113700). (jpa-00209849) (1984).
- [2] S. van Smaalen, “An elementary introduction to superspace crystallography”, *Zeitschrift für Kristallographie*, V 219, pp. 681-691, (2004).
- [3] T. Janssen, “On the lattice dynamics of incommensurate crystal phases,” *Journal of Physics C: Solid State Physics*, vol. 12, no. 24, pp. 5381-5392, (1979).
- [4] I. I. Nebola, Ya. A. Shteyfan, V. I. Sidey, A. F. Katanytsia, I. P. Studenyak, and I. M. Shkyrta, “Model research of phonon spectra of argyrodites family,” *Semiconductor Physics, Quantum Electronics & Optoelectronics*, vol. 21, pp. 134-138, doi: 10.15407/spqeo21.02.134, (2018).
- [5] I. I. Nebola, A. F. Katanytsia, I. M. Shkyrta, J. M. Pozho, and Yu. O. Pal, “Modification of phonon spectra of Ag 7 GeSe 5 I and Cu 7 GeSe 5 I crystals with different partial population of crystallographic orbits,” *International Journal of Science and Engineering Investigations*, vol. 10, no. 112, pp. 56-60, (2021).

# Track 9

Nanosensors, Nanodevices and Functional Systems

## Tellurene electronics and beyond

W. Wu<sup>1</sup>\*

1) *Purdue University, USA*

\* wenzhuowu AT purdue.edu

The development of wearable sensors for continuous monitoring of biomarkers is a promising alternative to the costly tools currently used in healthcare. Two-dimensional (2D) materials exhibit high sensitivity to physiology-relevant signals. However, few studies report 2D materials-based wearable sensors, primarily due to the intrinsic limitations of related materials that render them poor performance for sensing. Ongoing efforts in 2D materials also face difficulty scaling up due to restrictions on the synthesis conditions and stability. I will discuss our recent progress in developing tellurene-based wearable sensors with multiple modalities for continuously monitoring physiological and mental states. We show that wearable sensors based on tellurene, an emerging 2D semiconductor with intriguing properties, hold substantial promise for addressing the challenges of implementing 2D materials wearable sensors with high sensitivity and specificity. We aim to leverage our platform to fill the gaps in developing clinically applicable 2D materials-based wearable sensors.

---

**KEYWORDS:** Tellurene, 2D semiconductors, Nanoelectronics, Wearable sensors, Digital health

## The development of multi-pixel field emission x-ray devices

J. Yeow<sup>1</sup>\*

*1) University of Waterloo, Canada*

\* jyeow AT uwaterloo.ca

The first concept of multi-source Computed Tomography (CT) systems originated in the 1980s, and opened the way to innovative system concepts in X-ray and computed tomography. Multi-source CT systems offer promising opportunities in system performance. In addition, multi-source X-ray radiographic systems are widely studied, namely for X-ray stereographic imaging, X-ray tomosynthesis imaging, and inverse-geometry imaging. One significant benefit of the multi-source X-ray technology is the ability to fabricate the source array in various two-dimensional configurations. The more complicated distributive source topologies are designed to improve the sampling of projection data, to further improve both in-plane and depth imaging resolution within the constraints of the limited-angle acquisition of projection data. In multi-source systems, the X-ray sources are arranged in an array format, and each source is launched individually. However, current X-ray generators are not suited for these systems because of their large size, huge power requirement, and slow response. This talk will focus on the field emission X-ray technology that enables to the realization of multi-source CT systems.

---

**KEYWORDS:** Field emission, X-ray, Carbon nanotubes

## Advanced electrochemical immunosensors for SARS-CoV-2 detection based on gold nanostructures and MXenes

A. Ramanaviciene<sup>1\*</sup>, K. Sobol<sup>2</sup>, V. Liustrovaite<sup>3</sup>, B. Brasiunas<sup>3</sup>, A. Popov<sup>3</sup>, O. Gogotsi<sup>4</sup>, A. Ramanavicius<sup>5</sup>, I. Iatsunskiy<sup>6</sup>

1) NanoTechnas - Center of Nanotechnology and Materials Science, Institute of Chemistry, Faculty of Chemistry and Geosciences, Vilnius University, Naugarduko St. 24, LT-03225 Vilnius, Lithuania

2) NanoTechnas - Center of Nanotechnology and Materials Science, Institute of Chemistry, Faculty of Chemistry and Geosciences, Vilnius University, Naugarduko St. 24, LT-03225 Vilnius, Lithuania, Lithuania

3) NanoTechnas - Center of Nanotechnology and Materials Science, Institute of Chemistry, Faculty of Chemistry and Geosciences, Vilnius University, Naugarduko St. 24, LT-03225 Vilnius, Lithuania

4) Materials Research Center, Y-Carbon Ltd, Kyiv, Ukraine

5) Department of Physical Chemistry, Institute of Chemistry, Faculty of Chemistry and Geosciences, Vilnius University, Vilnius, Lithuania

6) Adam Mickiewicz University, Poland

\* almira.ramanaviciene AT chf.vu.lt

Electrochemical immunosensors have emerged as critical analytical platforms across diverse applications, particularly in biomedical diagnostics. These bioanalytical systems offer remarkable sensitivity and efficiency, rapid response, and ease of miniaturization. The principal operation of an electrochemical immunosensor is the conversion of specific antigen-antibody interaction into a measurable electrical signal, proportional to analyte concentration in the sample. In recent years, nanomaterials have emerged as powerful tools to enhance the sensitivity of immunosensors by modulating the electroactive surface area, improving electron transfer kinetics, and ensuring better spatial orientation and activity of biomolecules at the nano-bio interface [1-4].

In this presentation, two label-free electrochemical immunosensors will be presented. The first immunosensor, based on a graphite rod electrode electrochemically modified with gold nanostructures and covalently immobilized SARS-CoV-2 spike (S) protein, was developed for the detection of specific anti-S antibodies. The impact of gold nanostructures on the performance of the immunosensor was evaluated. Additionally, the influence of non-specific interactions on the analytical signal was investigated, along with methods used to reduce such effects. The second immunosensor, based on a screen printed graphite electrode modified with MXenes and polydopamine, was developed for the detection of the SARS-CoV-2 S protein. MXenes have attracted significant attention as two-dimensional materials with unique chemical, electrical, and morphological characteristics that can improve the performance of electrochemical biosensors. Although MXenes and their composites show considerable promise in biosensor development, further systematic investigation is required to elucidate their specific advantages and optimize their performance in sensing applications. This research provides valuable insights into the application of various nanomaterials in electrochemical immunosensors for biomedical applications.

---

**KEYWORDS:** Electrochemical immunosensor, Gold nanostructures, MXenes, SARS-CoV-2 spike protein, Specific antibody

---

**ACKNOWLEDGEMENTS:** This project has received funding from the Research Council of Lithuania (LMTLT), agreement No [S-LL-24-2].

---

### REFERENCES

- [1] A. Popov, B. Brasiunas, K. Blazevic, A. Kausaite-Minkstimiene, A. Ramanaviciene. Ultra-sensitive electrochemical immunosensors for clinically important biomarker detection: Prospects, Opportunities, and Global Trends. *Current Opinion in Electrochemistry* 2024, 46, 101524.
- [2] B. Brasiunas, A. Popov, G. Kraujelyte, A. Ramanaviciene. The effect of gold nanostructure morphology on label-free electrochemical immunosensor design. *Bioelectrochemistry* 2024, 156, 108638.
- [3] S. Hideshima, Y. Ogata, D. Takimoto, Y. Gogotsi, W. Sugimoto. Vertically aligned MXene bioelectrode prepared by freeze-drying assisted electrophoretic deposition for sensitive electrochemical protein detection. *Biosensors and Bioelectronics* 2022, 207, 114141.
- [4] A. Popov, V. Lisyte, M. Sapauskiene, S. Ramanavicius, S. Zukauskas, N. Slekiene, I. Baginskiy, V. Zahorodna, O. Gogotsi, A. Kausaite-Minkstimiene, A. Ramanaviciene. MXene-based electrochemical glucose biosensors: comparative enhancement with Aquivion and Nafion. *Materials Today Nano* 2025, 32, 100712.

## Programmable DNA origami Micro-Nano assemblies for optomechanics and Raman sensing

D. D. R. Arce<sup>1\*</sup>, M. Benešová<sup>2</sup>, L. Pirker<sup>1</sup>, V. Protiva<sup>1</sup>, K. Cardos<sup>1</sup>, J. Kočíšek<sup>1</sup>, A. Jonáš<sup>2</sup>, L. Sala<sup>1</sup>

1) J. Heyrovský Institute of Physical Chemistry of the CAS, Czech Republic

2) Institute of Scientific Instruments of the CAS, Czech Republic

\* david.ruiz AT jh-inst.cas.cz

DNA nanotechnology has revolutionized nanoscale fabrication by enabling the precise and programmable assembly of structures with nanometric precision [1]. Its unparalleled structural versatility makes it an ideal platform for organizing objects into complex hybrid architectures. Extending this concept toward microscale offers an exciting opportunity to bridge nanoscale precision with microscale functionality without relying on top-down methods. However, the controlled bottom-up fabrication of such hybrid micron-sized assemblies remains a major challenge. Here, we present the fabrication of well-defined hybrid micro-nano assemblies with controlled geometry and functionality where the DNA origami serves simultaneously as a rigid mechanical bridge between distinct microparticles and as a multifunctional nano-breadboard for the site-specific placement of fluorophores, quantum dots, and metallic nanoparticles [2]. Leveraging this programmability, we fabricate heterodimer microparticle assemblies (Janus-type) by using chemically modified specific sequences at the termini of the 24-helix bundle (24HB) to enable selective conjugation via biotin-streptavidin interactions and click chemistry [3]. The resulting heterodimers exhibit structural integrity, and selective DNA-mediated coupling is confirmed through fluorescence and transmission electron microscopy, revealing precise localization of the 24HB interlinks bridging the components. Moreover, these assemblies demonstrate robust mechanical stability under optical trapping, showing stable 2D and 3D confinement and orientation-dependent behavior arising from their intrinsic asymmetry. We further demonstrate hybrid micro-nano systems combining a polystyrene microsphere with a 50 nm gold nanoparticle linked by DNA origami, forming well-defined plasmonic nanogaps that enhance localized electromagnetic fields for surface-enhanced Raman spectroscopy (SERS). Beyond Raman or optical trapping applications, the modularity of this platform establishes DNA origami as a structural interface for coupling microscale manipulation with nanoscale plasmonic functionality [4]. This approach opens new opportunities for reconfigurable nanoplasmonic assemblies, optomechanical probes, and programmable photonic systems for sensing and spectroscopy.

---

**KEYWORDS:** DNA origami, Optical tweezers, RAMAN

---

**ACKNOWLEDGEMENTS:** This work has been funded by a grant from the Programme Johannes Amos Comenius under the Ministry of Education, Youth and Sports of the Czech Republic, reg. num. CZ.02.01.01/00/22\_010/0013757, NanoMove and by The Czech Science Foundation project Nanophotonics with hybrid DNA origami structures (grant No. 24-11503S).

---

### REFERENCES

- [1] P. W. K. Rothmund, “Folding DNA to create nanoscale shapes and patterns,” *Nature*, vol. 440, p. 297, Mar. 2006, [Online]. Available: <http://dx.doi.org/10.1038/nature04586>
- [2] A. Kuzyk *et al.*, “DNA-based self-assembly of chiral plasmonic nanostructures with tailored optical response,” *Nature*, vol. 483, no. 7389, pp. 311-314, 2012, doi: 10.1038/nature10889.
- [3] D. D. Ruiz Arce *et al.*, “Optomechanical Probes with Tailored Material and Shape Asymmetry Assembled Using DNA Origami,” *Nano Lett.*, vol. 26, no. 6, pp. 2080-2088, Feb. 2026, doi: 10.1021/acs.nanolett.5c05354.
- [4] K. Tapio, A. Mostafa, Y. Kanehira, A. Suma, A. Dutta, and I. Bald, “A Versatile DNA Origami-Based Plasmonic Nanoantenna for Label-Free Single-Molecule Surface-Enhanced Raman Spectroscopy,” *ACS Nano*, vol. 15, no. 4, pp. 7065-7077, Apr. 2021, doi: 10.1021/acsnano.1c00188.

## Advanced nanocomposite materials for high-performance hybrid sensors: Tuning selectivity for environmental and biomedical applications

O. Lupan<sup>1\*</sup>, O. Lupan<sup>2</sup>, M. Brinza<sup>2</sup>, S. Schröder<sup>3</sup>, D. Litra<sup>4</sup>, C. Lupan<sup>2</sup>, R. Nagpal<sup>5</sup>, M. Sugihara<sup>6</sup>, N. Magariu<sup>2</sup>, T. Strunskus<sup>7</sup>, R. Ameloot<sup>6</sup>, T. Ameri<sup>8</sup>, R. Adelung<sup>9</sup>

1) Technical University of Moldova, Republic of Moldova

2) Center for Nanotechnology and Nanosensors, Department of Microelectronics and Biomedical Engineering, Faculty CIM, Technical University of Moldova, 168 Stefan cel Mare str., MD-2004, Chisinau, Republic of Moldova, Republic of Moldova

3) Institute for Material Science Functional Nanomaterials, Kiel University, Germany

4) Department of Microelectronics and Biomedical Engineering, Technical University of Moldova Chisinau, Republic of Moldova, Republic of Moldova

5) Center for Nanotechnology and Nanosensors, Department of Microelectronics and Biomedical Engineering, Faculty CIM, Technical University of Moldova, 168 Stefan cel Mare str., MD-2004, Chisinau, Republic of Moldova, India

6) Centre for Membrane Separations, Adsorption, Catalysis, and Spectroscopy, University of Leuven, Oude Markt 13, 3000 Leuven, Belgium, Belgium

7) Faculty of Engineering Christian-Albrechts Universität Zu Kiel Kiel, Germany, Germany

8) Department of Materials Science, Chair for Composite Materials, Faculty of Engineering, Kiel University, Germany, Germany

9) Department of Materials Science, Chair for Functional Nanomaterials, Faculty of Engineering, Kiel, Kaiserstraße 2, D-24143 Kiel, Germany, Germany

\* lupanoleg AT yahoo.com

The demand for high-precision sensing in environmental monitoring and biomedical diagnostics has accelerated the development of multifunctional sensors fabricated using diverse approaches, composite nanomaterials, and advanced tuning processes. Considering the vast array of possibilities, a primary point of interest lies in nanocomposite materials and their integration into hybrid sensors designed to address specific challenges within environmental and biomedical niches and various biomarkers [1].

Previous studies have demonstrated significant potential for metal-oxide based gas sensors and tuning them by either functionalizing with various nanoparticles, and/or by coating them with polymers [2] and metal-organic frameworks [3] to enhance their sensitivity and selectivity for target analytes. Notably, the potential of TiO<sub>2</sub> coated with PV<sub>4</sub>D<sub>4</sub> polymer has been established, where samples were tuned via AgAu nanoparticles functionalization [4]. Furthermore, thermal annealing of the polymer transitioned the coating into a ring-to-cage structure, significantly increasing selectivity towards targeted analytes. Thus, a two-in-one sensor with a dual-response was obtained which responded as n-type for hydrogen and p-type for carbon dioxide with responses of up to 230% and 130 % respectively, [4] showcasing its versatility for multi-gas detection. In addition, research has focused on ZIF-71-coated, Al-doped CuO-based hybrid gas sensors [5]. These studies showed that this specific combination responded to n-butanol by up to 11% at 200 °C and to hydrogen gas by up to 61% at 250 °C, exhibiting excellent repeatability and durability. Furthermore, tests under various relative humidity levels showed that MOF-ZIF-71-coated CuO:Al possesses enormous potential for stable detection of targeted gases, [5] indicating the possibility of developing humidity-tolerant devices that remain stable over extended periods of operation.

Thus, in this paper, several sensors are presented to substantiate the potential of composite materials in detecting various biomarkers and target analytes for different industries, with emphasis on various tuning processes and the thermal annealing of various architectures. This paper explores the strategic design and fabrication of composite-based gas sensors, focusing on the synergistic effects achieved through advanced tuning processes and the resulting enhancements in molecular selectivity and sensitivity. Ultimately, our findings underscore the transformative role of hybrid nanocomposites in establishing a new generation of robust, multifunctional sensing platforms capable of meeting the rigorous environmental and clinical monitoring.

**KEYWORDS:** Hybrid sensors, Biomedical, Polymer

**ACKNOWLEDGEMENTS:** Acknowledgements. This work was partially funded through the 'Young Researchers' project, code 25.80012.5007.34TC, by the National Agency for Research and Development of Moldova at the Technical University of Moldova.

### REFERENCES

- [1] O. Lupan, M. Brinza, S. Schröder, N. Ababii, T. Strunskus, B. Viana, T. Pauporté, R. Adelung, F. Faupel, Sensors Based on Hybrid Materials for Environmental, Industrial and Biomedical Applications. In Proceedings of the 2024 IEEE 14th International Conference Nanomaterials: Applications and Properties (NAP); IEEE, September 8 2024; pp. MTF09-1-4.
- [2] O. Lupan, M. Brinza, J. Piehl, N. Ababii, N. Magariu, L. Zimoch, T. Strunskus, T. Pauporte, R. Adelung, F. Faupel, *et al.* Influence of Silsesquioxane-Containing Ultra-Thin Polymer Films on Metal Oxide Gas Sensor Performance for the Tunable Detection of Biomarkers. *Chemosensors* 2024, 12, 76, doi:10.3390/chemosensors12050076.
- [3] O. Lupan, R. Nagpal, D. Litra, M. Brinza, M. Sugihara, R. Ameloot, S. Railean, T. Ameri, R. Adelung, S. Schröder, *et al.* Hybrid Nanomaterials for Biomedical Sensors. In 7th International Conference on Nanotechnologies and Biomedical Engineering. (ICNBME 2025); V. Sontea, I. Tiginyanu, S. Railean, Ed.; Springer, Cham: Chişinău, 2025; pp. 162-176 ISBN 978-3-032-06494-3.
- [4] M. Brinza, L. Schwäke, S. Schröder, C. Lupan, N. Ababii, N. Magariu, M. Chiriac, F. Faupel, A. Vahl, O. Lupan, Two-in-One Hybrid Sensor Based on PV<sub>4</sub>D<sub>4</sub>/AgAu/TiO<sub>2</sub> Structure for Carbon Dioxide and Hydrogen Gas Detection in Biomedical and Industrial Fields. *Biosensors* 2025, 16, 5, doi:10.3390/bios16010005.
- [5] R. Nagpal, M. Sugihara, C. Lupan, T. Tjardts, Meling-N. Lizarde; T. Strunskus; H. Qiu; R. Adelung; R. Ameloot; Lupan, O. ZIF-71-Coated CuO:Al with Enhanced Gas-Sensing Performance for n-Butanol and Hydrogen. *ACS Appl. Electron. Mater.* 2025, 7, 10198-10215, doi:10.1021/acsaelm.5c01659.

## Concepts and prospects of hybrid memristive-chemiresistive hydrogen gas sensors

T. Plecenik<sup>1\*</sup>, M. Patrnčiak<sup>2</sup>, M. Vidiš<sup>1</sup>, L. Staňo<sup>1</sup>, T. Roch<sup>1</sup>, L. Satrapinsky<sup>1</sup>, P. Ďurina<sup>1</sup>, I. Shpetnyy<sup>1,3</sup>

1) Centre for Nanotechnology and Advanced Materials, Faculty of Mathematics, Physics and Informatics, Comenius University Bratislava, Mlynská Dolina, 84248 Bratislava, Slovakia

2) Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská cesta 9, 84104 Bratislava, Slovakia

3) Sumy State University, Kharkivska Str. 116, 40007 Sumy, Ukraine

\* tomas.plececnik AT fmph.uniba.sk

Hydrogen is a promising energy carrier widely utilized in energy storage applications, chemical synthesis and other areas of industry. However, due to its high flammability, reliable and fast detection is crucial to ensure safety. Conventional H<sub>2</sub> gas sensors face challenges in sensitivity, selectivity, and integration with intelligent systems [1]. Recently, hybrid devices combining gas sensing and memristive memory, gasistors, have been proposed and explored [2,3]. The gasistor integrates a metal-oxide semiconductor gas sensor and a resistive-switching element (memristor) into a single crossbar cell, e.g. Pt/TiO<sub>2</sub>/Pt. Such devices simultaneously detect the presence of hydrogen gas and store the detection event in their resistive state. Thanks to their structure, they can be easily integrated into crossbar arrays for in-sensor computing and other neuromorphic applications. Here we explore gasistor design improvements enabling higher sensitivity, stability, reproducibility, as well as new functionality of these hybrid devices.

The originally proposed single cell gasistor [3] suffers from high limit of detection (> 1000 ppm H<sub>2</sub>), caused by the extremely high baseline resistance of the sensing part, and limited resistive switching performance. It has been shown that incorporation of large-scale nanoporous top Pt electrodes in this type of sensors decreases the baseline resistance and allows detection of very low (down to 3 ppm) H<sub>2</sub> concentrations [4]. However, this approach is not directly applicable to single cell gasistors since large electrode cross-section area leads to much higher resistive switching currents, deteriorates the switching repeatability and can even lead to transition from bipolar to unipolar resistive switching. To address this problem, a modular gasistor with separate gas sensing and resistive switching cells is proposed. Such configuration allows for independent optimization of the two cells to maximize their gas sensing and resistive switching performance, respectively. Moreover, the two cells can be connected in both parallel and series configuration, detecting either decreasing or increasing H<sub>2</sub> concentration events, respectively. Preliminary results further indicate that a memristor cell exhibiting analogue (continuous) resistive switching, when integrated into a gasistor, can function as an analogue memory element. In this configuration, the gasistor is able to encode in its resistive state not only the occurrence of increasing or decreasing H<sub>2</sub> concentration events, but also the corresponding maximum or minimum H<sub>2</sub> concentration reached during its operation.

---

**KEYWORDS:** Gas sensors, Hydrogen, Gasistor, Memristor

---

**ACKNOWLEDGEMENTS:** This work was supported by the Slovak Research and Development Agency under the contract No. APVV-21-0053 and by the Scientific Grant Agency of the Slovak Ministry of Education, Sciences, Research and Sport (Grant No. VEGA 1/0062/22).

---

### REFERENCES

- [1] J. S. Lee, J. Oh, J. Jun, J. Jang, “Wireless Hydrogen Smart Sensor Based on Pt/Graphene-Immobilized Radio-Frequency Identification Tag”, *ACS Nano* 9, 7783-7790 (2015).
- [2] M. Vidiš, M. Patrnčiak, M. Moško, A. Plecenik, L. Satrapinsky, *et al.*, “Gas-triggered resistive switching and chemiresistive gas sensor with intrinsic memristive memory”, *Sens. Act. B* 389, 133878 (2023).
- [3] P. Qiu, Y. Qin, L. Zhu, “Memristive gas sensor (gasistor) based on Ag/ordered TiO<sub>2</sub> nanorods/FTO sandwich structure for evaluation of ethanol concentration in mixed ambient”, *Sens. Act. B* 421, 136548 (2024).
- [4] M. Patrnčiak, M. Vidiš, L. Staňo, I. Shpetnyy, T. Roch, *et al.*, “Highly sensitive hydrogen gas sensor based on a capacitor-like Pt/TiO<sub>2</sub>/Pt structure with large-scale nanoporous top electrode”, *Int. J. Hydrogen Energy* 99, 137-145 (2025).

## Challenges during the formation and application of molecularly imprinted polymers dedicated for the determination of large molecular weight analytes

A. Ramanavičius<sup>1,2\*</sup>, E. Mohsenzadeh<sup>3</sup>, E. Brazys<sup>4</sup>, V. Ratautaite<sup>3</sup>, G. Zvirzdine<sup>1</sup>, V. Liustrovaite<sup>5</sup>, R. Boguzaitė<sup>3</sup>, S. Bendinskaite<sup>6</sup>, G. Slaboseviciute<sup>1</sup>, G. Ruginyte<sup>1</sup>, A. Ramanaviciene<sup>7</sup>

1) Department of Nanotechnology, State Research Institute Center for Physical Sciences and Technology, Lithuania

2) MB Sensografa, Kiparisu 29, Vilnius Region, Lithuania

3) State Research Institute Centre for Physical Sciences and Technology (FTMC), Lithuania

4) Department of Physical Chemistry, Faculty of Chemistry and Geosciences, Vilnius University, Lithuania

5) NanoTechnas - Center of Nanotechnology and Materials Science, Institute of Chemistry, Faculty of Chemistry and Geosciences, Vilnius University, Naugarduko St. 24, LT-03225 Vilnius, Lithuania

6) Institute of Chemistry, Vilnius University, Naugarduko g. 24, LT-03225, Vilnius, Lithuania, Lithuania

7) NanoTechnas - Center of Nanotechnology and Materials Science, Institute of Chemistry, Faculty of Chemistry and Geosciences, Vilnius University, Naugarduko St. 24, LT-03225 Vilnius, Lithuania

\* arunas.ramanavicius AT chf.vu.lt

Early and accurate diagnosis of cancer is important biomedical issue. However, sometimes the duration and costs of diagnosis are rather high, require sophisticated bioanalytical equipment and should be performed by well-trained personnel. The application of sensors based on cheap artificial biological recognition elements could solve some recent technological problems in this research/technology direction [1-3]. Recently, molecularly imprinted polymers (MIPs) are gaining significant attention, because MIPs can replace antibodies and natural receptors, which most frequently are used for the determination of cancer biomarkers. In this presentation the ways in which MIPs can be formed directly on sensor electrochemical and/or surface plasmon resonance (SPR)-chip surface will be discussed. Proper and efficient polymerization is still challenging, therefore, before the polymerization is reasonable to apply mathematical and computational modelling to select suitable polymeric structure, which will properly interact with imprinted template/analyte. The selection of polymerization methods is also very important technological issue, which will be discussed during the presentation. For the deposition of MIP-based layers chemical and electrochemical methods could be applied. After polymer layer formation the next significant obstacle is 'mild' extraction of the template and formation of cavities complementary to selected biomarker. However, this technological step is not always easy and requires selection of proper eluent and extraction conditions suitable for this purpose. This task is especially complicated when we are trying to design MIP for large molecular weight cancer biomarkers. The next step, after the formation is the choice of the conditions for selective interaction of MIP with the biomarker, and the adaptation of sensitive analytical signal detection method. In our recent research the most frequently we are using electrochemical and surface plasmon resonance based analytical protocols. The advantage of electrochemical methods is that they can be used in optically nontransparent solutions, however the sensitivity of electrochemical methods is not always very high. This disadvantage could be eliminated or at least reduced by simultaneous application of surface plasmon resonance based analytical signal determination methods.

**KEYWORDS:** Molecularly imprinted polymers (MIPs), Surface plasmon resonance (SPR), Electrochemistry, Biomarker

**ACKNOWLEDGEMENTS:** This project has received funding from the Central Project Management Agency (CPVA), Project No 10-038-T-0330.

### REFERENCES

- [1] E. Mohsenzadeh, V. Ratautaite, E. Brazys, S. Ramanavicius, S. Zukauskas, D. Plausinaitis, A. Ramanavicius. Design of Molecularly Imprinted Polymers (MIP) using Computational Methods: a Review of Strategies and Approaches. WILEY Interdisciplinary Reviews Computational Molecular Science 2024 14:e1713. <https://doi.org/10.1002/wcms.1713>
- [2] E. Mohsenzadeh, V. Ratautaite, E. Brazys, S. Ramanavicius, S. Zukauskas, D. Plausinaitis, A. Ramanavicius. Application of computational methods in the design of molecularly imprinted polymers (review). Trends in Analytical Chemistry, 2024, 171, 117480. <https://doi.org/10.1016/j.trac.2023.117480>
- [3] E. Brazys, V. Ratautaite, E. Mohsenzadeh, R. Boguzaitė, A. Ramanaviciute, A. Ramanavicius, Formation of molecularly imprinted polymers: strategies applied for the removal of protein template (Review). Advances in Colloid and Interface Science, 2025, 337, 103386. <https://doi.org/10.1016/j.cis.2024.103386>

## Quantum sensing with NV centers in diamond: From nanoscale magnetometry to spin-wave imaging

A. Morales<sup>1</sup>\*

1) QZabre AG, Switzerland

\* andrea AT qzabre.com

NV centers in diamond are a leading platform for quantum sensing, offering atomic-scale spatial resolution and nanotesla-per-root-hertz magnetic field sensitivity under ambient conditions. Their spin-dependent photoluminescence, read out via ODMR, enables precise nanoscale magnetometry through Zeeman shifts of the ground-state spin sublevels.

In this contribution, I will present an overview of scanning NV magnetometry applied to complex magnetic materials. We first review the operating principles of NV-based quantum sensing and discuss recent technical advances in tip fabrication and stand-off distance minimization that have pushed spatial resolution below 50 nm. We then demonstrate scanning magnetometry results on archetypal multiferroic and ferrimagnetic materials. In BiFeO<sub>3</sub>, NV imaging reveals the sub 50 nm spin cycloid structure and its electrically controlled switching, providing quantitative stray-field maps of the antiferromagnetic order. In Bi:YIG, we image ferrimagnetic domain patterns with high contrast, exploiting the material's large magneto-optical response and low spin-wave damping.

Beyond static field imaging, we discuss NV-based magnetic noise spectroscopy, where spin relaxation measurements (T<sub>1</sub> relaxometry) probe GHz-frequency magnetic fluctuations. This approach enables the localization of domain walls and structural defects through their characteristic local enhancement of magnetic noise, offering a non-invasive probe of dynamic magnetism at the nanoscale.

Finally, we present NV-based spin-wave imaging. By detecting the evanescent microwave stray fields of propagating magnons, NV magnetometry resolves spin-wave wavefronts, dispersion relations, and mode selectivity via controlled sensor-sample distance tuning. Together, these capabilities position NV-center quantum sensing as a uniquely comprehensive tool for the nanoscale investigation of magnetic materials and spintronic devices.

---

**KEYWORDS:** BiFeO, Quantum sensing, Nanoscale magnetism, NV centers, Diamond

## MTJ-based artificial neuron suitable for fully analog machine learning

A. Slavin<sup>1\*</sup>, V. Tyberkevych<sup>1</sup>, S. Louis<sup>1</sup>

*1) Oakland University, USA*

\* slavin AT oakland.edu

Magnetic tunnel junctions (MTJs) are nanoscale spintronic devices composed of two ferromagnetic layers separated by an insulating barrier. MTJs are CMOS-compatible and widely used commercially in magnetic memory and sensor technologies, with over  $10^8$  devices manufactured annually. In this work, we demonstrate a practical analog artificial neuron by pairing a spin-valve/magnetic tunnel junction (SV/MTJ) device with an NMOS transistor. This SV/MTJ-nMOS neuron supports fully analog machine learning and is compatible with conventional electronic systems and neural network architectures.

In a recent theoretical study [1], it was shown that an SV/MTJ device can function as an artificial neuromorphic device replicating fundamental behaviors observed in biological neurons, such as short spike generation, response latency, synaptic integration, refraction, inhibition, adaptation, and spike-train generation. By integrating this SV/MTJ device with an NMOS transistor, both input and output signals become voltage-based. This configuration allows straightforward implementation of synaptic weights through voltage-controlled amplifiers, thus enabling seamless integration into fully analog neural networks.

To validate system-level performance, we constructed a three-neuron SV/MTJ-nMOS neural network in LTspice program, complete with supporting circuitry [2]. A feedforward backpropagation algorithm was employed, performing all learning and synaptic weight adjustments entirely in the analog domain using spike timing (time-encoded signals). An example of realization of an XOR logic gate, a standard neural network benchmark, was used to assess learning effectiveness. After approximately 30 training epochs, the network reliably converged, performing XOR classification successfully. The complete training cycle required less than 2  $\mu$ s of simulation time. These results confirm the potential of the SV/MTJ-nMOS artificial neuron circuit for fast, low-power, fully analog machine learning, compatible with standard electronic design and established neural network frameworks.

---

**KEYWORDS:** Magnetic tunnel junction (MTJ), Artificial neuron, Analog machine learning

---

**ACKNOWLEDGEMENTS:** This work was supported in part by the Oakland University Foundation.

---

### REFERENCES

- [1] S. Louis, H. Bradley, C. Trevillian, A. Slavin and V. Tyberkevych, "Spintronic Neuron Using a Magnetic Tunnel Junction for Low-Power Neuromorphic Computing," *IEEE Magnetics Letters* 15, 4500705, 1, (2024). doi: 10.1109/LMAG.2024.3484957.
- [2] S. Louis, H. Bradley, A. Litvinenko and V. Tyberkevych, "A Physics-Based Circuit Model for Magnetic Tunnel Junctions", arXiv preprint arXiv:2503.20813 (2025).

## Synthetic molecular recognition architectures for intelligent electrochemical sensing

U. Prentice<sup>1\*</sup>, D. Plausinaitis<sup>1</sup>, E. Vaicekauskaite<sup>1</sup>, A. Ramanavičius<sup>2,3</sup>

1) Vilnius University, Lithuania

2) Department of Nanotechnology, State Research Institute Center for Physical Sciences and Technology, Lithuania

3) MB Sensografa, Kiparisu 29, Vilnius Region, Lithuania

\* urte.prentice AT chgf.vu.lt

Selective molecular recognition remains one of the central challenges in the development of next-generation chemical and biosensing technologies, particularly for applications requiring operation in complex biological, pharmaceutical, and environmental matrices. Molecularly imprinted polymers (MIPs) have emerged as robust synthetic recognition materials capable of mimicking biological affinity systems while offering superior physicochemical stability, lower production costs, and compatibility with scalable sensor fabrication technologies.

This work discusses recent advances in electropolymerized MIP-based electrochemical sensing systems utilizing conducting polymer interfaces for selective analyte recognition. Particular emphasis is placed on polypyrrole-based molecular imprinting strategies and electrochemical transduction architectures enabling enhanced selectivity, sensitivity, and operational stability [1]. Previous studies demonstrated the successful application of molecularly imprinted polypyrrole layers for selective electrochemical detection of melamine, urine, and other biologically relevant compounds, highlighting the importance of polymer morphology, imprinting efficiency, and nanostructured modifications in sensor performance [2-5].

The work further examines how electrochemical deposition methods, conducting polymer engineering, and interfacial modification strategies contribute to the development of miniaturized and low-power analytical systems. Electrochemical and quartz crystal microbalance-based characterization approaches are discussed as effective tools for evaluating adsorption behavior, binding affinity, and recognition-layer dynamics in MIP architectures [3, 4].

Recent developments indicate that intelligently engineered MIP interfaces can support highly selective detection in complex matrices while remaining compatible with portable, wearable, and distributed sensing technologies. Emerging opportunities involving hybrid electrochemical platforms, intelligent signal processing, and autonomous sensing frameworks are also considered, particularly in relation to healthcare diagnostics, food safety assessment, and environmental monitoring applications [5].

These advances position molecular imprinting technologies as a promising platform for future intelligent sensing infrastructures integrating synthetic molecular recognition with scalable electrochemical analytical systems.

---

**KEYWORDS:** Molecularly imprinted polymers, Electrochemical sensors, Conducting polymers, Selective molecular recognition

---

### REFERENCES

- [1] E. Brazys, V. Ratautaite, B. Brasiunas, A. Ramanaviciene, L. Rodríguez, A. Pinto, D. Milea, U. Prentice, A. Ramanavičius, Molecularly Imprinted Polypyrrole-Based Electrochemical Melamine Sensors. *Microchemical Journal* 2024, 199, 109890. <https://doi.org/10.1016/j.microc.2024.109890>
- [2] V. Ratautaite, Samukaite-U. Bubniene; D. Plausinaitis; R. Boguzaitė; D. Balciunas; A. Ramanaviciene; G. Neunert; Ramanavičius, A. Molecular Imprinting Technology for Determination of Uric Acid. *International Journal of Molecular Sciences* 2021, 22, 5032. <https://doi.org/10.3390/ijms22095032>
- [3] G. Kaspute, D. Plausinaitis, V. Ratautaite, E. Vaicekauskaite, A. Ramanavičius, U.A. Prentice, Comparative Study of Molecularly Imprinted Polypyrrole Architectures for Electrochemical Quartz Microbalance-Based Method Development for Geraniol Adsorption. *Polymers* 2026, 18, 804. <https://doi.org/10.3390/polym18070804>
- [4] G. Kaspute, D. Plausinaitis, V. Ratautaite, E. Vaicekauskaite, V. Bucinskas, A. Ramanavičius, U. Prentice, Overcoming Template Surface Blocking: Geraniol Adsorption Studies Guiding MIP-Based Sensor Design. *Int. J. Mol. Sci.* 2025, 26, 11454. <https://doi.org/10.3390/ijms262311454>
- [5] J. Sarvutiene, U. Prentice, S. Ramanavičius, A. Ramanavičius, Molecular imprinting technology for biomedical applications, *Biotechnology Advances* 2024, 71, 108318. <https://doi.org/10.1016/j.biotechadv.2024.108318>

## Atomic and molecular layer deposition strategies for gas separation: Applications in membranes and sensing

M. Bechelany<sup>1</sup>\*

*1) CNRS/European Institute of Membranes, France*

\* mikhael.bechelany AT umontpellier.fr

Atomic Layer Deposition (ALD) and Molecular Layer Deposition (MLD) are two highly controlled thin-film deposition methods that have gained significant attention for the functional modification of porous materials used in gas separation processes. Their unique capability to build highly conformal coatings with angstrom-level precision enables precise engineering of membrane surfaces, pore architectures, and hybrid organic-inorganic interfaces. Through the controlled adjustment of surface chemistry, mechanical response, and effective pore size, ALD and MLD open new routes for tuning gas transport behavior and improving selectivity in both dense and porous separation systems.

In this presentation, we will highlight recent progress in the application of ALD and MLD across different classes of gas separation membranes, including inorganic, polymer-based, and mixed-matrix systems. Representative examples from our research will illustrate how modifications achieved via ALD/MLD can enhance membrane performance by improving selectivity, operational stability, and interfacial integration. Particular emphasis will be placed on the rational design of pore structures and hybrid coatings, which provide deeper insight into gas transport phenomena at the nanoscale.

Finally, we will address the current limitations and future opportunities associated with scaling up ALD and MLD technologies for membrane and sensor fabrication. The presentation will emphasize their growing potential in advancing next-generation gas separation solutions for clean energy production, carbon capture, and industrial gas purification.

---

**KEYWORDS:** Atomic layer deposition, Molecular layer deposition, Gas-separation membranes, Conformal coatings, Gas sensing

---

### REFERENCES

- [1] Journal of Membrane Science (2020), 596, 117701
- [2] Journal of Materials Chemistry A, 2023,11, 12202-12213
- [3] Advanced Materials Technologies (2024), 9, 2302081
- [4] Surfaces and Interfaces (2025), 62, 106181
- [5] Journal of Environmental Chemical Engineering (2025), 13, 116455
- [6] Coordination Chemistry Reviews, (2025), 541, 216836.

## From batch to continuous: Scalable microwave polyol synthesis of metallic nanoparticles

M. Salvador<sup>1\*</sup>, Y. F. Afonso<sup>1</sup>, C. Díaz-Ufano<sup>1</sup>, A. Santana-Otero<sup>1</sup>, A. Van Zomeren<sup>2</sup>, S. Bertran-Llorens<sup>2</sup>, V. Beni<sup>3</sup>, S. Veintemillas-Verdaguer<sup>1</sup>, M. D. P. Morales<sup>1</sup>

1) Instituto de Ciencia de Materiales de Madrid, ICMM/CSIC, C/Sor Juana Inés de la Cruz 3, 28049, Madrid, Spain

2) The Netherlands Organisation for Applied Scientific Research (TNO), P.O.Box 15, 1755 ZG, Petten, Netherlands

3) RISE Research Institutes of Sweden, Södra Grytsgatan 4, Norrköping SE 60223, Sweden

\* m.salvador AT csic.es

Metallic nanoparticles based on copper, iron, and nickel are compelling candidates for next-generation conductive inks, printed electronics, and magnetically functional materials, offering high performance at significantly lower cost than noble metals. However, their synthesis is typically hindered by oxidation susceptibility, reliance on hazardous reducing agents, and limited scalability.

We present a microwave-assisted polyol platform in which ethylene glycol acts as both solvent and reducing agent, eliminating external reductants and enabling reactions in air within minutes. Lignin, sourced from lignocellulosic biomass as a circular-economy byproduct, is incorporated as a bio-derived capping agent that simultaneously controls particle size and protects against oxidation across all three metal systems.

For copper, the platform delivers tunable particle sizes from ~47 to 800 nm, with the process transferring to a continuous-flow microwave reactor at production rates of ~5 g h<sup>-1</sup> and >95% reaction efficiency. Lignin-stabilized Cu nanoparticles show no detectable oxidation after nine months in air, and after sintering at 150 °C reach conductivities of 10<sup>5</sup>-10<sup>6</sup> S m<sup>-1</sup>, compatible with flexible substrates. For iron, zero-valent Fe nanoparticles (~ 70 nm) are obtained with saturation magnetization of 158 A·m<sup>2</sup>/kg, demonstrating robust room-temperature ferromagnetism. For nickel, introducing lignin together with preformed seeds reduces particle size from 730 to 239 nm while preserving a saturation magnetization consistent with metallic *fcc* Ni.

Together, these results establish microwave-polyol chemistry as a versatile, sustainable, and scalable route to Cu, Fe, and Ni nanomaterials for emerging applications in printed electronics and magnetic functional devices.

---

**KEYWORDS:** Microwave-assisted synthesis, Polyol process, Metallic nanoparticles, Conductive inks, Continuous-flow synthesis

## Core-shell Au@PEtOx-PBuOx colloids with tunable LCST transition for thermally switchable optical applications

O. Yeshchenko<sup>1</sup>, L. Daoud<sup>2</sup>, O. Fedotov<sup>1\*</sup>, P. Khort<sup>1</sup>, O. Krupka<sup>2</sup>

1) Faculty of Physics, Taras Shevchenko National University of Kyiv, Ukraine

2) University of Angers, France

\* oles.fedotov AT gmail.com

Hybrid nanostructures containing a noble metal core with polymer shell are the basis for the creation of “smart” materials with controllable properties. Such systems allow the adjustment of optical properties by external influence, which is of great importance for nanotechnology. Among such materials, polymers with lower critical solution temperature (LCST), capable of reversible phase transition upon heating, attract special attention. Poly(2-oxazolines) are promising polymers for such systems due to their high biocompatibility and the possibility of precise control of the phase transition temperature. However, the synthesis of stable hybrid nanosystems with sharp switching optical response in specific temperature ranges, in particular physiological ones, remains a difficult task. Here we show that our synthesized nanoparticles with a gold core and a shell of PEtOx-stat-PBuOx statistical copolymers act as thermosensitive optical absorptive switches with a tunable phase transition temperature. We found that increasing the proportion of the hydrophobic component PBuOx from 0 to 0.3 allows lowering the LCST point from 81°C to 17°C, reaching a biologically relevant 37°C at  $x=0.19$ . The phase transition is accompanied by compression of the polymer shell and subsequent aggregation of particles, which leads to a pronounced red shift and increase in the intensity of the localized surface plasmon resonance (LSPR) peak. The sensitivity of this hybrid nanosystem to structural changes is confirmed by SERS experiments, which demonstrate an enhancement of the Raman scattering intensity due to plasmon interaction during thermal cycling. The above-mentioned nanosystems are the basis for the creation of thermo-optical devices and sensors. The ability of the system to accurately respond to temperature variation near human body temperature makes these nanoparticles extremely promising for biomedical applications, in particular for in vivo diagnostics.

---

**KEYWORDS:** Gold nanoparticles, Nanobiosensors, Poly(2-oxazolines), LCST, LSPR

---

**ACKNOWLEDGEMENTS:** The work is supported by National Research Foundation of Ukraine (project 2025.07/0024)

## MoS<sub>2</sub>/PANI composite-based photoluminescence sensor for selective sensing of dimethoate pesticide

D. Panda<sup>1,1\*</sup>, K. P. Rao<sup>1</sup>

1) University of Delhi South Campus, New Delhi, India

\* dpanda AT electronics.du.ac.in

This study explores the development of a sensitive and selective sensing nanocomposite for detecting a widely used organophosphate pesticide called dimethoate. It poses significant environmental and health risks due to its high toxicity and persistence in agricultural products. To address these concerns, we developed a novel MoS<sub>2</sub> QDs/PANI nanocomposite and employed a photoluminescence technique to detect dimethoate. The MoS<sub>2</sub> QDs/PANI nanocomposite was synthesized in a single-step process and characterized using XRD, UV-visible, photoluminescence (PL), TEM, and FTIR techniques. The nanocomposite demonstrated selective detection of dimethoate which is one among other pesticides. Utilizing the PL approach, the sensing nanocomposite achieved a detection limit (LOD) of 1 nM and a linear range (LR) of 1-30 nM. The relative standard deviation (RSD) for metal ion interference was 3 % and 5 % for actual raw samples, indicating that, the nanocomposite has high specificity and stability. Additionally, the sensing nanocomposite exhibited a 5 % RSD for repeatability, confirming its reliability. The sensing parameters of the MoS<sub>2</sub>/PANI nanocomposite were compared with existing literature, highlighting its superior performance. This novel nanocomposite offers a promising solution for effective and reliable dimethoate detection, contributing to improved food safety and environmental protection.

---

**KEYWORDS:** Pesticide, Nanocomposite, MoS<sub>2</sub>, QDs, Photoluminescence

---

**ACKNOWLEDGEMENTS:** The authors gratefully acknowledge financial support from the UGCDAE-CSR, Kalpakkam, India (Grant Ref. no.: CRS/2021-22/04/599) and partly funded by the Institution of Eminence (IoE), University of Delhi, Delhi, India under the faculty research programme (IoE/2024-25/12/FRP). The first author (Mr. Dhananjaya Panda) is thankful to Council of Scientific & Industrial Research (CSIR), India for providing SRF-DIRECT fellowship.

---

### REFERENCES

- [1] H.K. Gill, H. Garg, Pesticide: environmental impacts and management strategies, *Pesticides-toxic aspects* 8 (187) (2014) 10-5772.
- [2] A. Alengebawy, S.T. Abdelkhalek, S.R. Qureshi, M.Q. Wang, Heavy metals and pesticides toxicity in agricultural soil and plants: ecological risks and human health implications, *Toxics*. 9 (3) (2021) 42.
- [3] G. Aragay, F. Pino, A. Merkoçi, Nanomaterials for sensing and destroying pesticides, *Chem. Rev.* 112 (10) (2012) 5317-5338.
- [4] Q. Dong, Q. Wei, Z. Tang, Molybdenum Disulfide (MoS<sub>2</sub>): an Emerging Multifunctional Nanomaterial for Sensing and Removal of Agricultural Contaminants, *ACS. Agric. Sci. Technol.* (2024).
- [5] Y. Wang, S. Sun, Y. Liu, Y. Zhang, J. Xia, Q. Yang, TiO<sub>2</sub> coupled to predominantly metallic MoS<sub>2</sub> for photocatalytic degradation of rhodamine B, *J. Mater. Sci.* 55 (2020) 12274-12286.

## Nanowire and nanoaperture probes of quantum turbulence in superfluid helium

P. Danylchenko<sup>1</sup>\*, Š. Midlik<sup>1</sup>, T. Šamožil<sup>2,3</sup>, A. Gheorghe<sup>1</sup>, S. Harašta<sup>1</sup>, D. Schmoranzer<sup>1</sup>

1) Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

2) CEITEC, Brno University of Technology, Brno, Czech Republic

3) Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic

\* petrdanil1997 AT gmail.com

Liquid helium ( $^4\text{He}$ ) is an essential quantum fluid and an important platform for studying macroscopic quantum phenomena at low temperatures. In its superfluid phase, helium supports so called quantum turbulence composed of quantized vortices with a core size of approximately 1 Å. Understanding the system on the quantum scale requires the development of nanoscale detector architectures.

In this work, we investigate superconducting Nb-Ti nanowires and fabricated silicon nitride nanoaperture-based structures as probes of quantum turbulence and Josephson oscillations in superfluid helium. Nanowires with characteristic dimensions on the order of hundreds of nanometers provide a sensitive platform for detecting vortex-induced dissipation and vortex interaction with oscillating structures, as well as the description of turbulent flows including in the superfluid counterflow regime. In parallel, we have developed and are working to employ nanoaperture arrays to realize superfluid  $^4\text{He}$  quantum interference devices (SHeQUIDs), where two helium reservoirs are weakly coupled via the nanostructured constrictions at temperatures starting below the superfluid transition.

One limitation in the current state of the art is the lack of local, scalable detectors capable of resolving effects present in superfluid helium with high precision at mesoscopic length scales. We show that nanowire-based sensors provide enhanced spatial sensitivity to turbulence-induced changes in the superfluid  $^4\text{He}$  environment compared to conventional micron-scale probes. In addition, nanoaperture SHeQUID devices will enable novel phase gradient meters to be integrated in superfluid flow experiments as well as unparalleled gyroscopy via the Sagnac effect.

Our results show improved sensitivity in comparison with previously used sensor architectures, enabled by the reduced dimensions and scalability of nanofabricated devices rather than a fundamentally new detection principle.

More broadly, our results show that nanostructured devices are powerful instruments for exploring the vast landscape of physical phenomena related to vortex dynamics and quantum turbulence.

---

**KEYWORDS:** Superfluid helium, SHeQUID, NEMS, Quantum turbulence

---

**ACKNOWLEDGEMENTS:** This work was supported by the Grant Agency of the Czech Republic (GACR), project No. 24-12253S. We acknowledge CzechNanoLab Research Infrastructure (ID 90251), supported by MEYS CR.

## Fano-enhanced fiber sensor using a gold nanodisc plasmonic array

I. Gorbov<sup>1</sup>\*, S. Korposh<sup>1</sup>, A. Lapchuk<sup>2</sup>, F. He<sup>1</sup>, S. Erdody<sup>1</sup>, H. Wang<sup>1</sup>

1) University of Nottingham, United Kingdom

2) Institute for Information Recording, NAS of Ukraine, Ukraine

\* ivan.gorbov AT nottingham.ac.uk

Optical fibre sensors (OFS) are widely used due to their high flexibility, miniature size, and immunity to electromagnetic interference. Localised surface plasmon resonance (LSPR) is attractive for OFS as it can measure the refractive index (RI) of surrounding medium, providing wavelength-encoded information in the reflected signal [1-3]. Relatively simple structures (nanoparticles, nanoholes, and disc arrays) deposited on the tip of the OFS, which can detect changes in the refractive index through shifts in the LSPR peak wavelength, were recently demonstrated [1-4]. However, in most cases, such structures have a simple broad plasmonic resonance that can't provide enough sensitivity for real applications. The sensitivity can be considerably increased by using Fano resonance which is fundamentally sensitive to changes in the environment because it is an interference phenomenon between two modes [5].

In this work, Fano-enhanced localized surface plasmon resonance of the periodical structure of a thin (50-60 nm) gold nanodisc array was studied. The sensitivity of an optical fiber sensor (OFS) based on such a periodical structure was simulated for two deposition cases: (i) nanodiscs embedded into the polymer deposited on the fiber tip and (ii) nanodiscs directly deposited on the tip. The fiber sensor was described as a periodic orthogonal structure of nanodiscs array deposited on the substrate with RI=1.496 according to the used fibre specification. 3D electrodynamic simulations were performed using the finite-difference time-domain (FDTD) method with the Lumerical FDTD Solutions Software. The simulation of one period of gold disc array with various thicknesses and radii (100 nm, 150 nm and 200 nm) deposited on fibre tip at various side-to-side interparticle distances has demonstrated the appearance of Fano resonance when nanodisc radius exceeds 150 nm. It results in the appearance of an additional reflection peak. It was shown that for the range of 1.3 - 1.4 RI, the sensitivity of 500 nm/RI for case (i) and 510 nm/RI for case (ii) can be reached for nanodiscs array with 200 nm radius and 50 nm thickness. The analysis of the field distribution at the observed reflection peaks shown presence of dipole and quadrupole modes, which results in Fano resonance observed on the absorption spectrum. Optical fibre sensors modified with an ultra-thin gold nanodisc metasurface were fabricated using a transfer process, and a sensitivity of 396 nm/RIU was experimentally confirmed for the case (i).

---

**KEYWORDS:** Optical fibre sensor, Refractive index sensor, LSPR, Nanodisc array, Fano resonance

---

**ACKNOWLEDGEMENTS:** This research was supported by the British Academy and the University of Nottingham through the Researchers at Risk Fellowships Programme (Grant RaR\100182).

---

### REFERENCES

- [1] H. Zhu, X. Wang, Y. Chen, X. Rao, Y. Qi, and Hua Yang, "Plasmonic refractive index sensor of a hexagonal close-packed gold nanodisk array coupled with a gold thin film," *J. Opt. Soc. Am. B*, 42, 1251-1257 (2025).
- [2] I. Gorbov, S. Korposh, A. Lapchuk, Seung-Woo Lee, Sandor Erdody, "Optimizing LSPR-based optical fibre refractive index sensor based on solid and hollow gold nanospheres," *Sensors and Actuators A: Physical*, 388, 116473 (2025).
- [3] V. Andrei, Kabashin, Vasyi G. Kravets and Alexander N. Grigorenko, "Label-free optical biosensing: going beyond the limits", *Chem. Soc. Rev.*, 52, 6554-6585 (2023).
- [4] L. Liu, S. S. Korposh, D. Gomez, *et al.*, "Localised plasmonic hybridisation mode optical fibre sensing of relative humidity", *Sensors & Actuators: B. Chemical* 353, 131157 (2022).
- [5] Z.E.A. Mohamed, S. Elshahat, A.M. Abd-Elnaiem, *et al.*, "Sensing performance of Fano resonance induced by the coupling of two 1D topological photonic crystals", *Opt Quant Electron*, 55, 943 (2023).

## Pesticides detection through fluorescent aminosilane-coated zno nanoparticles

L. Casoli<sup>1</sup>\*

1) University of Rome Tor Vergata, Italy

\* lorenzo.casoli AT gmail.com

Triazole fungicides are widely employed in agriculture to protect crops, herbs, and fruits; however, their extensive use raises concerns regarding environmental persistence and potential risks to human health [1]. Conventional analytical methods for pesticide detection, such as high-performance liquid chromatography, provide high sensitivity but often require expensive instrumentation, complex sample preparation, and long analysis times. In this work, we propose a rapid and sustainable fluorescence-based sensing strategy for the detection of penconazole, selected as a model triazole fungicide.

The sensing platform is based on ZnO nanoparticles, chosen for their low toxicity, biocompatibility, optical properties, and low production cost [2]. To improve colloidal stability and promote interaction with the analyte, the nanoparticles were functionalized with N-(2-aminoethyl)-3-aminopropyltrimethoxysilane (AEAPTMS). The methoxy groups of the silane undergo hydrolysis and condensation reactions with hydroxyl groups naturally present on the ZnO surface, forming stable Zn-O-Si bonds and generating a thin organosilane coating around the nanoparticles [3]. The exposed terminal amino groups reduce aggregation in aqueous media and provide active sites for interaction with penconazole molecules.

Surface modification was confirmed by IR spectroscopy, while UV-Vis measurements were employed to evaluate the stability and dispersibility of ZnO@AEAPTMS suspensions in hydrophilic solvents over time. Fluorescence measurements were then carried out by progressively adding penconazole to stable aqueous dispersions of the functionalized nanoparticles. Emission spectra were recorded upon excitation at 365 nm over a concentration range between 0 and 10 ppm.

The fluorescence intensity increased with increasing penconazole concentration up to approximately 3 ppm, after which a plateau was observed. The obtained trend suggests a concentration-dependent interaction between the analyte and the functionalized ZnO surface, supporting the potential use of ZnO@AEAPTMS nanocomposites as fluorescent nanosensors for pesticide detection.

Overall, this approach represents a promising alternative to conventional analytical techniques, combining sensitivity, simplicity, and sustainability for the monitoring of triazole pesticide residues in aqueous environments. L. Casoli (1), C. Ricci (1), G.A. Bracchini (1), A. Conti (1), I. Fabrizi (1), E.M. Bauer (2), A. Lembo (1), L. Gontrani (1), M. Carbone (1) (1) STARTNETICS, Department of Chemical Science and Technologies, University of Rome Tor Vergata. (2) Institute of Structure of Matter-Italian National Research Council (ISM-CNR)

---

**KEYWORDS:** ZnO nanoparticles, Coatings, Nanosensors, Fluorescence, Pesticide detection

---

### REFERENCES

- [1] V. S. Brauer, C. P. Rezende, A. M. Pessoni, R. G. De Paula, K. S. Rangappa, S. C. Nayaka, V. K. Gupta, F. Almeida, "Antifungal agents in agriculture: friends and foes of public health", *Biomolecules*, 9(10), 521 (2019).
- [2] L. Gontrani, E. M. Bauer, L. Casoli, C. Ricci, A. Lembo, D. T. Donia, S. Quaranta, & M. Carbone, "Inulin-Coated ZnO Nanoparticles: A Correlation between Preparation and Properties for Biostimulation Purposes", *Int. J. Mol. Sci.* 25(5), 2703 (2024)
- [3] N. Khurana, P. Arora, A. S. Pente, K. C. Pancholi, V. Kumar, C. P. Kaushik, & S. Rattan, "Surface modification of zinc oxide nanoparticles by vinyltriethoxy silane (VTES)" *Inorg. Chem. Commun.* 124, 108347 (2021)

## Sensor performance of hydrogel-based Gold/Carbon quantum dot nanocouples with metal enhanced fluorescence

A. Isler<sup>1</sup>\*, İ. E. Sümer<sup>1</sup>, Z. C. C. Ozdil<sup>1</sup>, F. Şahin<sup>1</sup>, V. Can<sup>1</sup>

1) Yeditepe Universtiy, Turkey

\* aleyna.isler AT std.yeditepe.edu.tr

Carbon quantum dots (CQDs) are a rapidly growing class of carbon-based nanomaterials known for their tunable fluorescence, biocompatibility, and rich surface functionality [1]. CQDs have been widely used for fluorescence-based detection of biomolecules, ions, and environmental analytes due to their rapid response, high sensitivity, and ease of surface modification [2]. In hydrogel-CQD systems, the hydrogel provides a hydrated three-dimensional network that improves nanoparticle dispersion and facilitates analyte diffusion while maintaining mechanical stability [3]. Immobilizing CQDs within hydrogels also enhances signal reproducibility, long-term stability, and localized fluorescence readout compared with colloidal systems [3,4]. By combining CQD fluorescence with the soft and permeable nature of hydrogels, these composites show strong potential for biomedical diagnostics, environmental monitoring, and portable sensing applications [4]. Coupling CQDs with gold nanoparticles enhances fluorescence through the metal-enhanced fluorescence (MEF) effect, leading to stronger emission than pristine CQDs. This enhancement arises from plasmonic interactions between gold nanoparticles and CQDs, highlighting the potential of Au/CQD nanostructures for sensitive optical sensing platforms [5]. In this study, poly(acrylic acid-co-acrylamide) hydrogels incorporating CQDs synthesized via a solid-state method were prepared at concentrations of 0-2.5% v/v to evaluate their functional properties. In parallel, CQDs synthesized in the presence of chloroauric acid ( $\text{HAuCl}_4 \cdot 3\text{H}_2\text{O}$ ) were incorporated at the same concentrations to investigate the effect of metal-enhanced fluorescence on emission behavior. The hydrogels were characterized in terms of rheological properties and fluorescence response. Rheological analysis showed a concentration-dependent decrease in mechanical strength with increasing nanoparticle content. For CQD-containing samples, increasing the concentration to 2.5% v/v reduced the storage modulus ( $G'$ ) from approximately 13,000 Pa to 2,000 Pa, corresponding to a 6-7 fold decrease. A more pronounced reduction was observed for Au/CQD hydrogels, where  $G'$  decreased to approximately 270 Pa at the same concentration, indicating a stronger weakening effect in the presence of Au. Fluorescence analysis also revealed a concentration-dependent decrease in emission intensity for both systems. As the concentration increased from 0.1% to 2.5% v/v, fluorescence intensity decreased by approximately 17 fold for CQD and 28-fold for Au/CQD. At 0.1% v/v, Au/CQD samples exhibited approximately 1.25 fold higher fluorescence intensity than CQD-only samples. This comparison highlights the influence of gold nanoparticles on the overall functional performance of the hydrogel system for potential biomedical sensing applications.

**KEYWORDS:** Fluorescence sensing, Hydrogel composites, Carbon quantum dot, Metal-Enhanced fluorescence

### REFERENCES

- [1] B. Sen and H. Sarma, “Carbon quantum dots as multifunctional nanomaterials for sustainable optoelectronic biosensing and green photonics,” *Commun. Mater.* (2026).
- [2] X. Li, M. Rui, J. Song, Z. Shen, and H. Zeng, “Carbon and graphene quantum dots for optoelectronic and sensing applications,” *Adv. Funct. Mater.*, 25, 4929-4947 (2015).
- [3] Y. Wang, T. Lv, K. Yin, N. Feng, X. Sun, J. Zhou, and H. Li, “Carbon dot-based hydrogels: Preparations, properties, and applications,” *Small*, 19, 2370119 (2023).
- [4] X. Zhao, Q. Lang, L. Yildirim, *et al.*, “Photoluminescent hydrogels for biosensing and bioelectronics,” *Adv. Mater.*, 28, 510-534 (2016).
- [5] V. Can, B. Onat, E. S. Cirit, F. Sahin, and Z. C. Canbek Ozdil, “Metal-enhanced fluorescent carbon quantum dots via one-pot solid state synthesis for cell imaging,” *ACS Appl. Bio Mater.*, 6, 1798-1805 (2023).

## Posters

T9-19

E-POSTER

### Thermal switching of photoluminescence of MoS<sub>2</sub> 2D quantum dots hybridized with colloidal Au@PEtOx core-shell nanoparticles

O. Yeshchenko<sup>1\*</sup>, P. Khort<sup>1</sup>, S. Golovynskyi<sup>2</sup>, O. Fedotov<sup>1</sup>, I. Golovynska<sup>2</sup>, O. Krupka<sup>3</sup>

1) Faculty of Physics, Taras Shevchenko National University of Kyiv, Ukraine

2) College of Physics and Optoelectronic Engineering, Shenzhen University, China

3) University of Angers, France

\* oleg.yeshchenko AT knu.ua

We study the thermo-induced morphological transformations and optical switching phenomena in colloid solution of nanohybrids, consisting of luminescent MoS<sub>2</sub> monolayer quantum dots (2D QDs) and Au@PEtOx core-shell nanoparticles (NPs) with a gold core and a shell of the thermoresponsive poly(2-ethyl-2-oxazoline) (PEtOx) polymer with a conformational lower critical solution temperature (LCST) phase transition. The binding of MoS<sub>2</sub> QDs to the PEtOx shell was confirmed through a combination of UV-Vis absorption, photoluminescence (PL), and Raman scattering spectroscopies. PEtOx exhibits a characteristic LCST phase transition behavior, undergoing conformational changes from a hydrophilic to a hydrophobic state upon heating. The effect of LCST transition in the PEtOx polymer shell on the MoS<sub>2</sub> QDs PL upon heating and reverse cooling was investigated in detail. Upon heating, the passing through the LCST point is accompanied by a step-like increase in the PL intensity with its subsequent sharp quenching. This sharp dependence of the PL intensity at LCST was attributed to be the result of the action of several physical mechanisms: the shrinking of the polymer shell during the phase transition, the NPs aggregation driven by the increased hydrophobicity of polymer shell, and the plasmonic PL enhancement of MoS<sub>2</sub> QDs in the Au core field.

In comparative studies of the MoS<sub>2</sub> QDs / PEtOx and MoS<sub>2</sub> QDs / Au@PEtOx NPs systems, the LCST point for PEtOx polymer bound to the Au core in Au@PEtOx NPs is noticeably higher (80 °C) compared to bare PEtOx (65 °C). Furthermore, in MoS<sub>2</sub> QDs / Au@PEtOx NPs nanohybrid, the jump-like changes in the PL intensity occur in a much narrower temperature range ( $\Delta T = 6$  °C) and have a noticeably larger relative enhancement (20.5 %) compared to MoS<sub>2</sub> QDs / PEtOx with  $\Delta T = 15$  °C and a 12.6 % enhancement. Thus, the narrow temperature range and large PL intensity jump are physical characteristics making the MoS<sub>2</sub> QDs / Au@PEtOx NP nanohybrid highly potential for creating high-sensitive luminescent nanothermometers and switches for the application in nanophotonics, biology, and nanomedicine.

The presented hybrid nanosystem represents a promising model and its performance can be further optimized for future applications. In particular, tuning the QD/NP ratio to enhance the amplitude and to make narrower the temperature window of the LCST-related PL switching, as well as modifying the copolymer shell composition to shift the LCST toward physiological conditions.

---

**KEYWORDS:** MoS<sub>2</sub> QDs / Au@PEtOx NP nanohybrid colloid, Thermo-responsive polymer, Thermo-induced optical switching, Nanophotonics

---

**ACKNOWLEDGEMENTS:** The work is supported by National Research Foundation of Ukraine (project 2025.07/0024) and Erasmus+ program (project KA171-HED-EA74CEA1).

## The effect of nanowire formation on the surface of a Si p-i-n structure on their electrical properties

M. Kukurudziak<sup>1</sup>, E. Mastruk<sup>2</sup>, D. Koziarskyi<sup>2</sup>, I. Koziarskyi<sup>2</sup> \*

1) Rhythm Optoelectronics Shareholding Company, Ukraine

2) Yuriy Fedkovych Chernivtsi National University, Ukraine

\* i.koziarskyi AT chnu.edu.ua

Silicon nanostructured surfaces in the form of nanoporous layers or arrays of nanowires (NW) are effectively used in the manufacture of various types of detectors, in particular photodetectors based on *p-i-n* structures. Such layers allow for an increase in the effective radiation absorption area at the operating wavelength (which is particularly relevant in the near-IR region, where silicon has low absorption), an increase in the effective path length of radiation within the semiconductor, and a reduction in the surface reflectance.

Here, we have shown that by establishing the optimal depth of the nanostructured layer or the optimal length of the NW located in the doped  $n^+$ -region, it is possible to achieve more efficient radiation absorption without significant degradation of the dark current.

The Si *p-i-n* structures with NW were fabricated using diffusion-planar technology according to the process conditions described in [1]. Arrays of NW were formed by metal-assisted etching of silicon substrates in a mixture of hydrofluoric acid and hydrogen peroxide, with prior deposition of silver nanoparticles in aqueous mixtures of  $\text{AgNO}_3$  and HF. NW with a thickness of 30-40 nm and a length of approximately 200-230 nm were formed in a phosphorus-doped  $n^+$ -layer with a thickness of approximately 4.2-4.6  $\mu\text{m}$ . Planar samples were compared with samples containing an array of nanowires.

From the reverse *I-V* characteristics of the structures, it was established that the nanostructured samples nevertheless possessed a slightly higher dark current density:  $J_d = 78\text{-}82 \mu\text{A}/\text{cm}^2$  for planar structures and  $J_d = 81\text{-}94 \mu\text{A}/\text{cm}^2$  for nanostructured ones ( $V_{bias} = -100 \text{ V}$ ). For both types of samples, the activation energy at low ( $V_{bias} = -20 \text{ V}$ ) bias voltages was  $E_a = 0.56\text{-}0.57 \text{ eV}$ , indicating the dominance of the generation mechanism of current transport, and at high reverse voltages ( $V_{bias} = -100 \text{ V}$ ), the activation energy was  $E_a = 0.45\text{-}0.46 \text{ eV}$ , indicating the predominance of the generation mechanism in the space charge region with a contribution from tunneling through localized (trapped) states.

The depth of the donor energy levels (at low voltages) from which thermal generation of charge carriers occurs was  $\Delta E \approx 0.14 \text{ eV}$  for the nanostructured sample and  $\Delta E \approx 0.18 \text{ eV}$  for the planar sample. The determined energy level depth was  $\Delta E \approx 0.2 \text{ eV}$  for the nanostructured sample and  $\Delta E \approx 0.18 \text{ eV}$  for the planar sample. A slight change in the dark current without a change in the current transport mechanism indicates only a slight increase in the surface density of traps that induce additional surface generation. The conducted studies indicate the potential effective use of the investigated structures in the production of *p-i-n* photodiodes, which will allow for a significant increase in the detection efficiency and sensitivity of photodetectors with a minimal change in dark current; this is possible provided that NW are formed in the doped front layers.

---

**KEYWORDS:** Si p-i-n structures, Nanowires, Mechanism of current transport, Activation energy, Dark current

---

### REFERENCES

- [1] M. S. Kukurudziak, E. V. Mastruk, R. Yatskiv, I. P. Koziarskyi, and D. P. Koziarskyi, "Silicon pin photodiode with reduced crystallographic defect density and structured surface", *Journal of Physics D: Applied Physics*, 58 (16), 165106 (2025).

## Electrical properties of photosensitive heterostructures ITO/*n*-ZnFe<sub>2</sub>O<sub>4</sub>/*n*-CdTe

I. Orletskyi<sup>1</sup>, I. Koziarskyi<sup>1</sup>, M. Ilashchuk<sup>1</sup>, E. Mastruk<sup>1</sup>, D. Koziarskyi<sup>1</sup>\*, M. Koval<sup>1</sup>, H. Andrushchak<sup>1</sup>

1) Yuriy Fedkovych Chernivtsi National University, Ukraine

\* d.koziarskyi AT chnu.edu.ua

Thin films of zinc ferrite ZnFe<sub>2</sub>O<sub>4</sub> obtained by various technological methods are characterized by a band gap  $E_g \approx 1.9 - 2.1$  eV [1] and a high transmittance in the spectral region of visible radiation ( $T > 60\%$ ). The  $E_g$  values of the films, as well as their optical and electrical properties, determine their use in heterojunctions and heterostructures as front or buffer (when using a front film of transparent conductive oxide) layers.

ITO/*n*-ZnFe<sub>2</sub>O<sub>4</sub>/*n*-CdTe diode structures were fabricated by sequentially depositing ZnFe<sub>2</sub>O<sub>4</sub> thin films by spray pyrolysis and magnetron sputtering a film of transparent conducting oxide ITO (In<sub>2</sub>O<sub>3</sub>:Sn) onto the surface of plane-parallel CdTe crystalline plates. *n*-CdTe substrates with a specific electrical conductivity  $\sigma = 1.4$  fi·cm<sup>-1</sup>, electron concentration  $n = 8.75 \cdot 10^{15}$  cm<sup>-3</sup>, and Hall mobility  $\mu_H = 1000$  cm<sup>2</sup>·V<sup>-1</sup>·s<sup>-1</sup> (at  $T = 300$  K) were used.

The resistivity of *n*-ZnFe<sub>2</sub>O<sub>4</sub> films was  $\rho \approx 10^6$  fi·cm.

The diode properties of the structures are confirmed by the high current rectification ratio of  $\sim 2 \cdot 10^5$  at  $T = 296$  K and  $|V| = 1.0$  V. The analysis of *I-V*-characteristics measured in the temperature range  $T = 296 - 341$  K was carried out taking into account the profile of energy bands of the ITO/*n*-ZnFe<sub>2</sub>O<sub>4</sub>/*n*-CdTe heterostructure. It has been established that the energy barrier that determines the electrical properties of the heterostructure is formed in the near-surface region of *n*-CdTe. According to the estimate by extrapolation of the straight branches of the *I-V*-characteristics to the voltage axis, the barrier height  $q\phi_b = 1.1$  eV. A high value of  $q\phi_b$  leads to the formation of an inversion layer in *n*-CdTe, the presence of which significantly affects the current transfer mechanisms in the studied structures.

In the range of forward voltages  $3kT/q < V < 0.6$  V in ITO/*n*-ZnFe<sub>2</sub>O<sub>4</sub>/*n*-CdTe heterostructures, the recombination mechanism of current transfer with the participation of deep levels in the middle of the CdTe band gap  $E_C - 0.63$  eV dominates. A decrease in the barrier thickness with a further increase in the forward voltage causes electron tunneling from the CdTe conduction band into the conduction band of the ZnFe<sub>2</sub>O<sub>4</sub> film. The determined tunneling activation energy is  $\Delta E_t \approx 0.3$  eV, and it can be interpreted as the energy of the level in the conduction band of CdTe from which tunneling occurs  $\Delta E_t = E_t - E_C \approx 0.3$  eV. At reverse biases  $-1.3$  V  $< V < -3kT/q$ , the generation of electrons in the space charge region from deep energy levels  $E_C - 0.56$  eV in the CdTe band gap with their subsequent movement into the base region of the structure is decisive. An increase in the reverse voltage above 1.3 V leads to an avalanche multiplication of charge carriers in the strong electric field of the barrier region of the structure. ITO/*n*-ZnFe<sub>2</sub>O<sub>4</sub>/*n*-CdTe heterostructures are photosensitive and promising for use as visible radiation sensors.

---

**KEYWORDS:** Heterostructures, Thin films, ZnFe<sub>2</sub>O<sub>4</sub>, Mechanism of current transfer, Photosensitive

---

### REFERENCES

- [1] X. Wang, Y. Zhang, D. Jia, J. Wei, D. Hou, J. Tian, and T. Jiang, “Highly-porous CuFe<sub>2</sub>O<sub>4</sub>@ZnFe<sub>2</sub>O<sub>4</sub> yolk-shell heterostructure for photocatalytic reduction of nitrobenzene”, *Journal of Alloys and Compounds*, 994, 174717 (2024).

## Geometry-driven temporal signal encoding in TiO<sub>2</sub> gas sensors for neural network integration

P. Nemeč<sup>1\*</sup>, J. Klarák<sup>1</sup>, M. Predanocý<sup>1</sup>, M. Horský<sup>2</sup>, J. Škriniarová<sup>1</sup>, B. Hudec<sup>3</sup>

1) Institute of Informatics, Slovak Academy of Sciences, Bratislava, Slovakia, Slovakia

2) Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava, Slovakia

3) Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská cesta 9, 84104 Bratislava, Slovakia

\* pavol.nemec AT savba.sk

TiO<sub>2</sub>-based gas sensors are typically evaluated using scalar electrical parameters, such as resistance-based metrics or steady-state response at a given gas concentration. However, such scalar approaches inherently discard a significant portion of the information encoded in the temporal evolution of the sensor signal [1], [2].

This work introduces a geometry-driven interpretation of TiO<sub>2</sub> gas sensing, in which the sensor output is reinterpreted as a dynamic signal rather than a single measurement value. Nanostructured TiO<sub>2</sub> sensing elements with systematically varied contact and active-area geometries were designed and fabricated using electron-beam lithography. The use of electron-beam lithography enables the formation of submicron-scale structures and provides a pathway for systematic control of geometrical parameters, enabling controlled investigation and optimization [3].

Here, geometry is treated as a dual-function parameter that simultaneously defines the effective sensing area and modulates the kinetics of gas interaction processes, including adsorption, desorption, diffusion, and charge transport [3], [4]. As a result, different geometrical configurations can generate distinct temporal electrical signatures under identical gas exposure conditions.

Experimental measurements were performed for hydrogen in the concentration range of 50-10,000 ppm under controlled temperature conditions. The analysis focused on transient response characteristics, recovery behavior, and overall signal morphology. The results demonstrate that geometrical variations lead to reproducible and systematic differences in dynamic signal profiles, including cases where steady-state metrics fail to distinguish between sensor configurations.

To interpret these observations, a geometry-informed representation of the sensor response is proposed. This approach links structural parameters with steady-state and dynamic signal characteristics and enables the transition from scalar outputs to multidimensional feature vectors derived from temporal signal evolution. Within this framework, a sensor array composed of geometrically diverse elements can be interpreted as a hardware-defined feature extraction layer for subsequent neural network processing. Instead of assigning each sensor to a single input variable, the time-dependent responses themselves form the feature space for subsequent data analysis [2], [5]. The presented concept establishes a direct link between sensor design and data representation, enabling the co-design of sensing structures and machine learning models and opening a pathway toward gas sensing systems where nanostructured geometry directly encodes information for AI-based classification at the sensor level.

---

**KEYWORDS:** TiO<sub>2</sub> gas sensors, Hydrogen detection, Dynamic response, Temporal signal encoding, Neural networks

---

**ACKNOWLEDGEMENTS:** This work was supported by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09105-03-V02-00058 (NEURALSENS) and project Vega 2/0140/26 "Next-Generation Gas Sensors Integrating Advanced 2D Materials and Neural Networks for Enhanced Detection of Gases in the Environment".

---

### REFERENCES

- [1] M. A. Z. Chowdhury and M. A. Oehlschlaeger, "Artificial Intelligence in Gas Sensing: A Review," *ACS Sens.*, vol. 10, no. 3, pp. 1538-1563, Mar. 2025, doi: 10.1021/acssensors.4c02272.
- [2] J. Han, H. Li, J. Cheng, X. Ma, and Y. Fu, "Advances in metal oxide semiconductor gas sensor arrays based on machine learning algorithms," *J. Mater. Chem. C*, vol. 13, no. 9, pp. 4285-4309, Feb. 2025, doi: 10.1039/D4TC05220J.
- [3] P. Nemeč, I. Hotovy, V. Rehacek, and R. Andok, "TiO<sub>2</sub> sensoric structures with controlled extension of their active area by electron-beam lithography and reactive ion etching techniques," in *AIP Conference Proceedings*, vol. 2411, 060003, 2021. doi: 10.1063/5.0067745.
- [4] B. Hudec *et al.*, "Hydrogen sensing characteristics of TiO<sub>2</sub> thin films grown by atomic layer deposition using TTIP precursor with H<sub>2</sub>O vs. O<sub>3</sub> reactants," *Nanomaterials: Applications & Properties - 2023: 2023 IEEE 13th International Conference*.
- [5] N. N. Viet, P. H. Phuoc, L. V. Thong, N. V. Chien, and N. Van Hieu, "A comparative study of machine learning models for identifying noxious gases through thermal fingerprint measurements and MOS sensors," *Sens. Actuators A Phys.*, vol. 375, p. 115510, Sep. 2024, doi: 10.1016/j.sna.2024.115510.

## Extending the measurement range and accuracy of MagLev density systems through off-center imaging

E. Kara<sup>1\*</sup>, Y. Ö. Ömür<sup>2</sup>, N. E. Taşçılar<sup>2</sup>, Y. Oztürk<sup>2</sup>

1) Department of Mechatronics Engineering, Ege University, İzmir, Turkey

2) Department of Electrical and Electronics Engineering, Faculty of Engineering, Ege University, İzmir, Turkey

\* esrakar015 AT gmail.com

Magnetic levitation (MagLev) based applications are utilized across diverse fields, including industrial engineering, materials science, and biochemistry, due to their ability to enable contactless manipulation of organic and inorganic materials. Density measurement is one of the key applications of MagLev, which is based on determining density from the levitation height of diamagnetic or paramagnetic objects within a paramagnetic or diamagnetic fluid. Permanent magnet-based MagLev systems offer several advantages, including the ability to measure the density of one or more samples simultaneously, label-free measurement, and portability.

Rectangular prisms and cylindrical-shaped magnets with the same poles facing each other can be used in MagLev density measurement systems. However, especially in rectangular magnet geometries, magnetic levitation measurements are generally taken around the central symmetry axis of the magnets. On this central axis, aligned magnets generate a magnetic force primarily opposite to gravity, while other magnetic field components cancel due to symmetry. Accordingly, when the measurement axis shifts from the central axis, other components become non-zero, which changes the magnetic field gradient and thus the force. From another perspective, when measurements are taken only on the central axis, the number of samples that can be measured is limited due to the limited range of the imaging system. By considering these issues, it has been shown that shifting the measurement region from the central axis toward the edges increases both the number of measurable samples and the measurement accuracy by accounting for off-axis magnetic field components.

To theoretically analyze off-center measurements, magnetic field components were calculated for Anti-Helmholtz geometry magnets, and a measurement system was developed. A capillary tube placed between two rectangular magnets, an illumination module, a microcontroller with custom-designed Python-based software, an HQ camera with a lens, and a translation stage were utilized to develop the system. The camera system was shifted from the central axis toward the edges of the magnets, and the positions of microparticles with known densities were recorded.

Particles with an average density of 1.09 g/mL within an 82.5 mM Gadovist paramagnetic solution were used to confirm the theoretical calculations. A total of 297 samples were investigated while the system was laterally shifted by 21.5 mm from the central axis. The results indicate that, when only the magnetic forces along the central axis are considered, the maximum observed deviation was found to be in line with the theoretical calculations and was around 1 kg/m<sup>3</sup>. The maximum theoretical deviation found for different densities was 4.55 kg/m<sup>3</sup>.

---

**KEYWORDS:** Maglev, Magnetic field of rectangular magnet system, Density measurement, Magnetic levitation

---

### REFERENCES

- [1] Anil-M. Inevi, O. Sarigil, Y.C. Unal, H.C. Tekin, G. Mese, & Ozcivici, E. (2025). Magnetic levitation-based determination of single-nuclei density. *Biomaterials Advances*, 214581.
- [2] G. Bölükbaşı, S. Gümüş, Sabour-M. Takanlou, Sabour-L. Takanlou, Y. Öztürk, A.T. Vardarlı, ... & Güneri, P. (2025). Magnetic levitation-based density profiling for ex vivo differentiation of oral squamous cell carcinoma, oral epithelial dysplasia, and benign oral lesions. *Oral Surgery, Oral Medicine, Oral Pathology and Oral Radiology*.

## Electrochemical formation and sensory properties of polypyrrole/Ti<sub>2</sub>AlC nanocomposite films

Y. Horbenko<sup>1\*</sup>, O. Aksimtyeva<sup>1</sup>, A. Zhytskyi<sup>1</sup>, V. Kordan<sup>1</sup>

1) Ivan Franko National University of Lviv, Ukraine

\* Yuliia.Horbenko AT lnu.edu.ua

Polypyrrole (PPy) is one of the most widely studied conducting polymers due to its high electrical conductivity, environmental stability, and biocompatibility, enabling a broad range of practical applications, including corrosion protection, energy storage systems, biomedical technologies, and sensing devices [1-3]. Electrochemical deposition is a well-established method for fabricating PPy thin films. This technique enables precise control over the thickness and morphology of the resulting polymer layer by adjusting parameters such as the applied potential and deposition time. MAX phases, particularly Ti<sub>2</sub>AlC, are a class of highly conductive layered materials characterized by a unique combination of metallic and ceramic properties. Owing to their structure, which consists of strong Ti-C bonds and relatively weaker Ti-Al bonds, these materials exhibit high electrical conductivity, excellent thermal and mechanical stability, and oxidation resistance. Despite these advantages, the influence of MAX phases on the properties of conducting polymers remains poorly explored. The present work aims to establish the conditions for the electrochemical deposition of PPy/Ti<sub>2</sub>AlC nanocomposite films onto optically transparent semiconductor electrodes and to study their sensing properties.

The PPy/Ti<sub>2</sub>AlC composite films were fabricated on glass substrates coated with a semiconducting SnO<sub>2</sub> layer using cyclic voltammetry. It was established that monomer electrooxidation occurs at 0.7 V vs. Ag/AgCl and results in the formation of uniform polymeric films. At -0.4 V, a cathodic peak appears, the intensity of which increases with the number of scan cycles, probably due to charge-accumulation processes driven by MXene-like layers, which increase electrical conductivity and the specific surface area of the composite films. The sample morphology was examined by scanning electron microscopy, while surface elemental analysis confirmed the incorporation of Ti<sub>2</sub>AlC into the polymer matrix. Compared to pristine PPy films, the PPy/Ti<sub>2</sub>AlC nanocomposites exhibited enhanced optical absorption across the entire spectral range, along with a shift of the absorption maximum from 370 to 450 nm, attributed to  $\pi$ - $\pi^*$  transitions within the conjugated polymer backbone. It was found that the adsorption of organic solvent molecules significantly changes the surface resistance of the composite film, measured by the two-point method. Moreover, the incorporation of Ti<sub>2</sub>AlC particles considerably improves the sensitivity of polypyrrole by 5 times to acetone, and by 16 times to acetonitrile vapors.

---

**KEYWORDS:** Polypyrrole, MAX phase, Electrochemical deposition, Resistive sensors

---

### REFERENCES

- [1] A. Olad, A. Rashidzadeh, and M. Amini, “Preparation of polypyrrole nanocomposites with organophilic and hydrophilic montmorillonite and investigation of their corrosion protection on iron”, *Adv. Polym. Technol.*, 32(2), 21337 (2013).
- [2] M. S. Kim, J. H. Moon, P. J. Yoo, and J. H. Park, “Hollow polypyrrole films: Application for energy storage devices”, *J. Electrochem. Soc.*, 159(7), A1052 (2012).
- [3] E. N. Zare, T. Agarwal, A. Zarepour, and F. Pinelli, “Electroconductive multi-functional polypyrrole composites for biomedical applications”, *Appl. Mater. Today*, 24, 101117 (2021).
- [4] G. H. Jeong, G. R. Baek, T. F. Zhang, and K. H. Kim, “Max-phase Ti<sub>2</sub>AlC ceramics: Syntheses, properties and feasibility of applications in micro electrical discharge machining”, *J. Ceram. Process. Res.*, 17(10), 1116 (2016).
- [5] M. Li, K. Wang, J. Wang, D. Long, and Y. Liang, “Preparation of TiC/Ti<sub>2</sub>AlC coating on carbon fiber and investigation of the oxidation resistance properties”, *J. Am. Ceram. Soc.*, 101(11), 5269 (2018).

## Steady-state and high-speed switching behavior of dual silicon nanowire gate-all-around field effect transistors

A. Verma<sup>1\*</sup>, R. Nekovei<sup>1</sup>

1) Texas A&M University - Kingsville, USA

\* amit.verma AT tamuk.edu

We investigate the effects of various dielectric materials on the electronic performance of dual silicon-nanowire (SiNW) Gate-All-Around Field-Effect Transistors (GAAFETs). Building upon our previous research, this study evaluates both direct current (DC) characteristics and high-frequency switching dynamics across different dielectric substrates, including titanium dioxide (TiO<sub>2</sub>), tantalum pentoxide (Ta<sub>2</sub>O<sub>5</sub>), cerium oxide (CeO<sub>2</sub>), and aluminum oxide (Al<sub>2</sub>O<sub>3</sub>). FET structures with multiple active nanowire channels within the same device matrix can deliver higher currents than a single-channel device. Such structures are also relatively easy to fabricate compared to GAAFETs, in which the gate surrounds each individual channel [1]. Experimental results have shown the former structures to demonstrate outstanding performance [2]. Our previous work [3] demonstrated that within small GAAFET structures with 2 SiNWs as the active channels, and with gate-lengths of 50 nm, dielectric radius of 25 nm, and the edge-to-edge distance between the nanowires ranging from 5 nm to 10 nm, there is a substantial gain in overall drain current compared to a single SiNW channel. However, the gain is less than twice, and decreases with decreasing distance between the SiNWs. This is because the electronic coupling between the channels shields the gate, thereby reducing gate control.

An ensemble Monte Carlo (EMC) simulation of electron transport [3] serves as the basis for determining the device structure's electronic response. The EMC simulation uses a calculated band structure based on empirical Tight-Binding (TB). The lowest 4 conduction subbands are used within the EMC simulation. Electron-phonon scattering rates, through longitudinal acoustic and optical phonons, are calculated using first-order perturbation theory and Fermi's Golden Rule. These calculations also include inter-subband electron transfer.

The impact of multiple active SiNW channels within a shared dielectric matrix in a GAAFET configuration has been systematically examined. Although the aggregate drain current in this multi-channel architecture exceeds that of a single SiNW channel GAAFET, the channels exhibit substantial electrostatic coupling, resulting in lower current levels than isolated SiNW channels operating within independent GAA structures.

---

**KEYWORDS:** Gate-All-Around transistor, Field-Effect-Transistor, Silicon nanowire, Electron-Phonon scattering, Ensemble Monte Carlo

---

**ACKNOWLEDGEMENTS:** The authors acknowledge the generous use of supercomputing resources provided by the High-Performance Computing Cluster (HPCC) at Texas A&M University-Kingsville.

---

### REFERENCES

- [1] M. Wang, "A Review of Reliability in Gate-All-Around Nanosheet Devices," *Micromachines* (Basel), vol. 15(2), p. 269, 2024
- [2] H. Zhu, Q. Li, H. Yuan, H. Baumgart, D.E. Ioannou, and C.A. Richter, "Self-aligned multi-channel silicon nanowire field-effect transistors," *Solid-State Electronics*, vol. 78, p. 92, 2012
- [3] R. Nekovei and A. Verma, "Electronic Response of a Gate-All-Around Field Effect Transistor with Two Silicon Nanowires as Active Channels within the Same Insulator Matrix," 2025 IEEE 15th International Conference on Nanomaterials: Applications & Properties (NAP), pp. NNA02-1-NNA02-4, Bratislava, Slovakia, 2025

## Luminescent hydrogen peroxide sensor based on oxygen-deficient TbO<sub>2-x</sub> nanocrystals

O. Samoilo<sup>1</sup>\*, P. Maksimchuk<sup>1</sup>, V. Seminko<sup>1</sup>, S. Yefimova<sup>1</sup>, M. Lupan<sup>1</sup>, A. Onishchenko<sup>2</sup>, V. Klochkov<sup>1</sup>, G. Grygorova<sup>1</sup>

1) Institute for Scintillation Materials, NAS of Ukraine, Ukraine

2) Kharkiv National University of Radio Electronics, Ukraine

\* samoilovisma AT gmail.com

The development of efficient sensors for the detection of reactive oxygen species, particularly hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>), represents a critical objective in the fields of analytical chemistry and biomedical monitoring [1]. This research focuses on the unique sensory capabilities of oxygen-deficient terbium oxide (TbO<sub>2-x</sub>) nanoparticles, which offer a promising alternative to traditional rare-earth oxide platforms.

Stable aqueous solutions of these nanoparticles, characterized by an average size of approximately 20 nm and a cubic fluorite-type crystal structure, were successfully produced via colloidal synthesis methods. A key feature of these nanoparticles is the coexistence of terbium ions in both trivalent (Tb<sup>3+</sup>) and tetravalent (Tb<sup>4+</sup>) states, with the Tb<sup>3+</sup> fraction measuring approximately 33% as confirmed by X-ray photoelectron spectroscopy. Under UV excitation, the TbO<sub>2-x</sub> nanoparticles exhibit characteristic narrow-band luminescence, corresponding to the 4f–4f electronic transitions of the Tb<sup>3+</sup> ions. The sensory response is initiated upon the addition of hydrogen peroxide, which triggers a significant luminescence quenching, thereby enabling a "turn-off" detection mode. This quenching is primarily driven by the H<sub>2</sub>O<sub>2</sub>-induced oxidation of Tb<sup>3+</sup> to Tb<sup>4+</sup> occurring at the nanoparticle surface. Beyond simple intensity changes, the ratio between the emission bands at 617 nm (<sup>5</sup>D<sub>4</sub>→<sup>7</sup>F<sub>3</sub>) and 544 nm (<sup>5</sup>D<sub>4</sub>→<sup>7</sup>F<sub>5</sub>) demonstrates a linear correlation with the analyte concentration. Such a ratiometric sensing approach provides a built-in calibration mechanism that enhances measurement precision.

The developed sensor is effective across a wide concentration range from 0.25 mM to 400 mM. The adsorption kinetics of H<sub>2</sub>O<sub>2</sub> on the nanoterbia surface are most accurately modeled by the Temkin isotherm, suggesting a heterogeneous surface environment with varying adsorption energies. A distinct characteristic of this system is its irreversibility; the luminescence intensity does not recover after the sensing event due to the high standard redox potential of the Tb<sup>3+</sup>/Tb<sup>4+</sup> pair (+3.1 V), which prevents the spontaneous back-reduction of the cations.

The use of TbO<sub>2-x</sub> nanocrystals opens up new possibilities for the creation of luminescent H<sub>2</sub>O<sub>2</sub> sensors. Due to the linear dependence of the spectral line intensity ratio on the H<sub>2</sub>O<sub>2</sub> concentration, these nanoparticles ensure high measurement accuracy in ratiometric mode, making them promising for use in precision analytical and biomedical systems.

---

**KEYWORDS:** Terbium oxide nanoparticles, Hydrogen peroxide, Luminescent sensor, Luminescence quenching, Reactive oxygen species

---

**ACKNOWLEDGEMENTS:** This research was supported by National Research Foundation of Ukraine, Grant № 2025.07/0093.

### REFERENCES

- [1] J. Meier, E. M Hofferber, J. A Stapleton, N. M Iverson. "Hydrogen Peroxide Sensors for Biomedical Applications". Chemosensors 2019, 7, 64.

## Dual-mode luminescent sensing of H<sub>2</sub>O<sub>2</sub> using Eu<sup>3+</sup>-doped colloidal nanoceria

Y. Neuhodov<sup>1\*</sup>, P. Maksimchuk<sup>1</sup>, A. Onishchenko<sup>2</sup>, N. Kavok<sup>1</sup>, G. Dudetskaya<sup>1</sup>, Y. Kot<sup>3</sup>, S. Yefimova<sup>1</sup>, V. Seminko<sup>1</sup>

1) Institute for Scintillation Materials, NAS of Ukraine, Ukraine

2) Kharkiv National University of Radio Electronics, Ukraine

3) V. N. Karazin Kharkiv National University, Ministry of Education and Science of Ukraine, Kharkiv, Ukraine, Ukraine

\* e.i.neuhodov AT gmail.com

Reactive oxygen species (ROS) play a fundamental role in cellular physiology, acting as both essential signaling molecules and potential agents of oxidative stress [1]. Among various ROS, hydrogen peroxide (HP) has recommended itself as a key biological agent, being a ubiquitous and highly reactive cell signaling molecule that is essential for regulating numerous physiological processes.

The dual nature of HP makes the precise control and monitoring of its concentration imperative. While controlled levels of HP are necessary for normal cell signaling, fluctuating or excessive HP levels are linked to various pathological conditions, necessitating the development of sensors capable of real-time, in situ monitoring in complex biological systems. While organic fluorescent sensors offer high sensitivity, they often suffer from low photostability and irreversibility, which limits their use for tracking these dynamic fluctuations [2]. To overcome these limitations, this study proposes an inorganic sensor based on Eu<sup>3+</sup>-doped colloidal ceria nanoparticles (CeO<sub>2-x</sub>:Eu<sup>3+</sup>), which combine the unique redox activity of nanoceria with the stable luminescent properties of rare-earth ions.

The developed sensor operates in two distinct modes:

1. Turn-off Sensing. The addition of HP leads to the monotonic quenching of both the Ce<sup>3+</sup> (430 nm) and Eu<sup>3+</sup> (591 nm) luminescence bands. The quenching of Ce<sup>3+</sup> is caused by its oxidation to the non-luminescent Ce<sup>4+</sup> state by HP molecules adsorbed on the NP surface. In contrast, the quenching of Eu<sup>3+</sup> luminescence is attributed to hydroxyl groups formed during the catalytic decomposition of HP on the NP surface.
2. Ratiometric Sensing. The sensor allows for ratiometric detection by monitoring the ratio between the <sup>5</sup>D<sub>0</sub> → <sup>7</sup>F<sub>1</sub> (591 nm, symmetry-insensitive) and <sup>5</sup>D<sub>0</sub> → <sup>7</sup>F<sub>2</sub> (606 nm, symmetry-sensitive) transitions of Eu<sup>3+</sup>. The Ce<sup>3+</sup> → Ce<sup>4+</sup> oxidation process reduces the number of oxygen vacancies, which increases the local symmetry around Eu<sup>3+</sup> ions and subsequently increases the 591/606 nm intensity ratio. The CeO<sub>2-x</sub>:Eu<sup>3+</sup> nanoparticles provide a robust, multi-channel platform for HP sensing. The ability to perform ratiometric measurements enhances data reliability by minimizing the influence of environmental factors and equipment settings. Successful testing in cell media confirms the potential of these NPs for real-time HP monitoring in complex biological environments.

---

**KEYWORDS:** Ceria nanoparticles, Hydrogen peroxide, Redox activity, Ratiometric sensor

---

**ACKNOWLEDGEMENTS:** This research was supported by National Research Foundation of Ukraine, Grant № 2023.03/0050

### REFERENCES

- [1] B. Halliwell, J.M. Gutteridge, Free radicals in biology and medicine, fifth ed., Oxford University Press, Oxford, 2015.
- [2] M. Schäferling, D.B.M. Grögel, S. Schreml, "Luminescent probes for detection and imaging of hydrogen peroxide", *Microchim. Acta.*, 2011, 174, 1-18.

# Track 10

Nanomaterials for Energy and Environmental Technologies

## Transition metal dichalcogenide nanotubes: Engineering charge transport in perovskite solar cell devices

A. Laikhtman<sup>1\*</sup>, A. Zak<sup>2</sup>, A. Gajovic<sup>3</sup>, S. Dolic<sup>3</sup>, V. Kojic<sup>3</sup>

1) HIT-Holon Institute of Technology, Israel

2) Holon Institute of Technology, Israel

3) Rudjer Boskovic Institute RBI, Croatia

\* alexl AT hit.ac.il

Formamidinium lead-halide perovskites are among the most promising solution-processed photovoltaic absorbers, and their electronic performance can be further improved by integrating compatible low-dimensional semiconductors [1,2]. We examine transition-metal dichalcogenide (TMD) nanotubes, with emphasis on tungsten disulfide WS<sub>2</sub> nanotubes, as multifunctional additives for both the perovskite absorber and TiO<sub>2</sub> electron-transport architecture. WS<sub>2</sub> hollow nanotubes synthesized by a high-temperature vapor-gas-solid reaction were incorporated into formamidinium perovskite thin films, where solid-state impedance spectroscopy showed enhanced electrical conductivity without deterioration of optical properties [3]. In parallel, WS<sub>2</sub> and MoS<sub>2</sub> nanotubes were embedded in compact and mesoporous TiO<sub>2</sub> bilayers on fluorine-doped tin oxide and evaluated using various surface and electrochemical analysis methods. The nanotubes dispersed poorly in compact TiO<sub>2</sub> but integrated effectively within the mesoporous network while preserving visible transmittance and the TiO<sub>2</sub> band edge. Electrochemical and transport measurements indicate that WS<sub>2</sub> in mesoporous TiO<sub>2</sub> promotes interfacial charge separation, increases photocurrent, improves leakage blocking, and enhances key diode parameters, including shunt resistance, series resistance, and reverse saturation current [4,5]. By contrast, MoS<sub>2</sub> in the mesoporous layer degraded film integrity. Overall, the results identify WS<sub>2</sub> nanotubes as energy-level-compatible additives capable of improving charge transport in formamidinium perovskite films and optimizing TiO<sub>2</sub>-based electron-transport bilayers, offering a practical route to more efficient perovskite and photoelectrochemical devices.

**KEYWORDS:** WS<sub>2</sub> and MoS<sub>2</sub>, Nanotubes, Formamidinium perovskites, Charge transport, Perovskite solar cells

**ACKNOWLEDGEMENTS:** Ministry of Science, Education and Youth Croatia and the Ministry of iNNOVATION, Science and Technology of Israel: project Sol-HP-TMD-NanoComp. COST Action RenewPV CA21148, supported by European Cooperation in Science and Technology.

### REFERENCES

- [1] A. Kojima, K. Teshima, Y. Shirai, and T. Miyasaka, "Organometal Halide Perovskites as Visible-Light Sensitizers for Photovoltaic Cells," *J. Am. Chem. Soc.*, 131(17), 6050-6051 (2009).
- [2] M. M. Lee, J. Teuscher, T. Miyasaka, T. N. Murakami, and H. J. Snaith, "Efficient Hybrid Solar Cells Based on Meso-Superstructured Organometal Halide Perovskites," *Sci.*, 338(6107), 643-647 (2012).
- [3] S. Dolić, V. Kojić, A. Zak, A. Laikhtman, H. Mo, T. Čižmar, I. Erceg, L. Klobučar, K. Juraić, and A. Gajović, "Enhancing the Electrical Performance of Formamidinium Perovskites through WS<sub>2</sub> Nanotube Incorporation," *ACS Omega* 11(18), 26411-26420 (2026).
- [4] R. Tenne, L. Margulis, M. Genut, and G. Hodes, "Polyhedral and Cylindrical Structures of Tungsten Disulphide," *Nature*, 360, 444-446 (1992).
- [5] D. Tsikritzis *et al.*, "Engineering of the Perovskite/Electron-Transporting Layer Interface with Transition Metal Chalcogenides for Improving the Performance of Inverted Perovskite Solar Cells," *Sustainable Energy & Fuels*, 8, 2180-2190 (2024).

## Biomimetic interfaces in strain-driven photocatalysis

E. Coy<sup>1</sup> \*

*1) NanoBioMedical Centre, Adam Mickiewicz University, ul. Wszechnicy Piastowskiej 3, 61-614 Poznan, Poland*

\* coyeme AT amu.edu.pl

Nowadays, polydopamine (PDA) is a rather well-known biomimetic polymer with a vast range of applications. In this talk, I will explain the development of multifunctional catalysts using a mechanism we have termed interfacial temporal control. The research shows that the thickness of a polydopamine coating on zinc oxide tetrapods (ZnOT) determines the material's flexophotocatalytic selectivity, shifting the preference toward either oxidative or reductive pathways. The presentation will provide experimental evidence of a thickness-dependent efficient charge-transfer interface. We will show how a PDA configuration promotes the generation of hydroxyl radicals, which are highly effective at degrading organic pollutants. Conversely, we show that a different configuration functions as a capacitive electron sink. This physical change temporarily decouples the electron and hole pathways, thereby suppressing recombination and increasing hydrogen evolution rates. The presentation will further show that both processes are driven by the photo-flexoelectric effect in ZnOT structures, offering a reliable method for engineering catalysts with programmable selectivity for specific environmental and energy applications.

---

**KEYWORDS:** Flexoelectrics, Photocatalysis, Strain-driven, Water-Splitting

---

**ACKNOWLEDGEMENTS:** The authors thank the financial funding from the National Science Foundation of Poland (NCN) by the SONATA Grant UMO-2021/43/D/ST5/01116

## Learning exciton transport mechanisms in next generation materials from simulation based inference

S. Pressé<sup>1</sup>\*, S. Roberts<sup>2</sup>, T. Volek<sup>2</sup>, B. Nainggolan<sup>1</sup>

1) Arizona State University, Phoenix, AZ, USA

2) UT Austin, USA

\* spresse AT asu.edu

Singlet fission (SF) materials, which convert a single absorbed photon into two triplet excitons, are promising platforms for high-efficiency energy conversion, quantum sensing, and next-generation optoelectronic technologies. However, practical deployment remains limited by inefficient triplet transport and extraction, particularly across heterogeneous interfaces and silicon heterojunctions. Quantitative understanding of the microscopic transport mechanisms and kinetic parameters governing triplet motion in realistic SF materials is therefore essential for device optimization.

Learning these kinetic parameters is challenging because the underlying dynamics are highly nonlinear, particularly in the presence of processes such as singlet-singlet annihilation. Existing approaches often rely on spatially averaged measurements or simplified diffusion models that assume Gaussian exciton distributions at all times, limiting their ability to capture the non-Gaussian, multi-mechanism transport dynamics characteristic of SF materials. As a result, current methods provide limited quantitative insight into the microscopic mechanisms controlling triplet mobility and extraction.

Transient absorption microscopy (TAM) offers a direct route to overcome these limitations by enabling spatially and temporally resolved imaging of exciton populations following photoexcitation. In a typical TAM experiment, a tightly focused pump pulse generates singlet excitons that subsequently undergo transport and singlet-triplet interconversion. The resulting dynamics are probed using a time-delayed, co-focused probe pulse raster-scanned across the excitation region. Repeating these pump-probe measurements over a range of delay times produces quantitative, time-resolved maps of evolving exciton distributions.

To interpret these complex dynamics, we will present recently developed Bayesian inference frameworks to systems whose behavior is accessible only through simulation (in other words, whose likelihood can only be numerically reconstructed through simulation), as is the case for non-linear exciton transport in SF materials. In these systems, coupled nonlinear and spatially heterogeneous processes do not admit analytical likelihoods for purposes of inference. Our approach, relying on an adaptation of simulation-based inference (SBI), leverages simulations of candidate transport models and compares them directly with experimental observations to infer posterior probability distributions over model parameters. By recovering posterior distributions directly from TAM data, this framework enables quantitative identification of transport mechanisms and prediction of how perturbations, such as spatial heterogeneity in transport parameters, influence exciton dynamics and triplet extraction even quantifying anisotropic diffusion in perylenediimide crystals for the first time.

---

**KEYWORDS:** Transient absorption microscopy, Singlet fission materials, Bayesian inference, High-efficiency energy conversion, Next-generation optoelectronic technologies

---

**ACKNOWLEDGEMENTS:** Tanner Scott Volek, Sean Roberts (UT Austin); Bonfilio Nainggolan (ASU)

## Application of nickel iron layered double hydroxides/activated carbon (NiFe-LDH@AC) composite for preconcentration and removal of Cr and As from water systems

L. Nyaba<sup>1, 2\*</sup>, P. N. Nomngongo<sup>1, 2</sup>, B. P. Khunou<sup>1</sup>

1) Department of Chemical Sciences, University of Johannesburg, Doornfontein, Johannesburg 2028, South Africa

2) Department of Science and Innovation-National Research Foundation South African Research Chairs Initiative (DSI-NRF SARCH) in Nanotechnology for Water, University of Johannesburg, Doornfontein, Johannesburg 2028, South Africa

\* Inyaba AT uj.ac.za

A nickel-iron layered double hydroxides/activated carbon (NiFe-LDH@AC) composite was synthesised via hydrothermal assisted ultrasonic exfoliation and its structural properties and morphologies were characterised using various analytical characterization techniques. These include transmission electron microscopy (TEM), scanning electron microscopy coupled with energy dispersive spectroscopy (SEM-EDS), Fourier transform infrared (FT-IR) spectroscopy, Brunauer-Emmett-Teller (BET) and X-ray diffraction (XRD). The material was applied as an adsorbent for preconcentration and removal of As and Cr. The target analytes were quantified using inductively coupled plasma optical emission spectroscopy (ICP-OES). Under the optimal conditions, the preconcentration method was validated with respect to linearity, limits of detection (LOQ), accuracy, limits of quantification (LOQ) and precision. The linear ranges were 0.1-150 µg/L and 0.07-100 µg/L for As and Cr, respectively. The precision was investigated in terms of repeatability and reproducibility. The results were expressed in terms of relative standard deviation (%RSD) and the values were less than 5%. The LOD and LOQ ranged from 0.021-0.031 and 0.1-0.07 µg/L for As and Cr, respectively. Finally, the accuracy was validated by successfully analysing spiked samples and the recoveries ranged from 92.6-99.2%. The adsorbent was then explored for the removal of target analytes and adsorption capacities were 102 mg/g and 92.6 mg/g for As and Cr, respectively. The metal ions adsorption was evaluated using kinetics and isotherm models and the results followed pseudo second-order kinetics and Langmuir isotherms. Finally, the removal efficiency for spiked effluent wastewater samples ranged from 89.7-100%.

---

**KEYWORDS:** Adsorption, Layered double hydroxide, Wastewater

---

**ACKNOWLEDGEMENTS:** The authors send their sincere gratitude to the University of Johannesburg (Department of Chemical Sciences) and the National Research Foundation Thuthuka for their support through the facilities used in this study.

## Hollow carbon nanospheres vs resorcinol-formaldehyde nanospheres for adsorptive removal of emerging contaminants from water

N. J. Waleng<sup>1</sup>\*

*1) University of Johannesburg, South Africa*

\* ngwakowaleng AT gmail.com

### Abstract

The contamination of water systems by emerging pollutants has resulted in severe environmental and human health impacts. Consequently, there is a critical need to develop and engineer advanced nanomaterials for the effective adsorptive removal of these contaminants from water<sup>1</sup>. This study fabricated 3D hollow carbon nanospheres (HCNSs) utilizing a water-in-oil (W/O) microemulsion method<sup>2</sup>. The material was characterized by XRD, FTIR, N<sub>2</sub> adsorption-desorption, SEM, and TEM. The performance of HCNSs was assessed in comparison with resorcinol-formaldehyde hollow nanospheres (RF-HNSs), which is a carbon precursor for HCNS synthesis. The RF-HNSs exhibited significantly lower adsorption efficiency compared to HCNSs. Using HCNSs, adsorption isotherm analysis showed maximum adsorption capacities for all analytes. Furthermore, the equilibrium data were best described by Langmuir, indicating monolayer adsorption. Kinetic analysis indicated a mixture of pseudo-first order and pseudo second-order. The Dubinin-Radushkevich (D-R) model revealed a mixture of chemisorption and physisorption. The developed adsorption method was applied to real water samples (river water samples), achieving removal efficiencies of up to 98%. In addition, the adsorbent could be regenerated with methanol and reused up to 5 times without significant loss in the performance. Overall, the HCNSs exhibited excellent reusability and great potential as an effective adsorbent for efficient removal of selected emerging pollutants from aquatic environments.

---

**KEYWORDS:** Pharmaceuticals, Adsorption, Central composite design, Hollow carbon nanospheres

---

**ACKNOWLEDGEMENTS:** The authors would like to thank the University of Johannesburg for allowing us to utilise their laboratory spaces to conduct our research. The authors are also thankful to the National Research foundation Postdoctoral grants (South Africa) for their financial support.

---

### REFERENCES

- [1] References
- [1] Abd-ElH. Fattah, R.M. Kamel, A. Maged, & Kharbish, S. (2025). Harnessing clays and clay composites for efficient removal of pharmaceutical contaminants from water: A review. *Frontiers in Scientific Research and Technology*.
  - [2] A.L.S. Vieira, R.S. Ribeiro, A.R.L. Ribeiro, A.M. Ribeiro, A.M. Silva, Hollow carbon spheres for diclofenac and venlafaxine adsorption. *Journal of Environmental Chemical Engineering*, 10(3), 107348 (2022).

## Green-synthesized $\text{Bi}_{19}\text{S}_{27}\text{I}_3$ -PEG nanohybrids for efficient Chromium(VI) water treatment

M. M. Frutos<sup>1\*</sup>, M. Viera<sup>1</sup>, I. Aguiar<sup>1</sup>, M. E. P. Barthaburu<sup>2</sup>

1) Area Radioquímica, DEC, Facultad de Química, Udelar, Uruguay

2) Departamento de Desarrollo Tecnológico, CURE, Udelar, Uruguay

\* maiaam AT fq.edu.uy

$\text{Bi}_{19}\text{S}_{27}\text{I}_3$  is a novel bismuth-based chalcogenide with promising optical and electronic properties, making it a potential candidate for photocatalytic applications. Nanostructures of this material can be synthesized in various morphologies, with nanorods, nanorolls and nanoflowers being the most commonly reported. Recent efforts in sustainable water treatment have focused on developing efficient photocatalysts, and  $\text{Bi}_{19}\text{S}_{27}\text{I}_3$  nanorolls, with high surface area have shown potential in pollutant degradation [1,2]. In this study, we evaluate the photocatalytic performance of  $\text{Bi}_{19}\text{S}_{27}\text{I}_3$ -PEG hybrid nanomaterials for the reduction of chromium (VI). The hybrid material was synthesized using a green hot-injection method with water as the solvent. The concentration of polyethylene glycol (PEG) was found to influence the resulting morphology, yielding, nanorolls, round nanoparticles or mixed structures at PEG:Bi molar ratios of 0.5:1, 1:1, and 2:1. Additionally, an extended reaction time (270 min vs. 5 min) enhanced both crystallinity and morphological uniformity.

Photocatalytic experiments were systematically carried out under a range of pH conditions and chromium (VI) concentrations to evaluate the performance of the  $\text{Bi}_{19}\text{S}_{27}\text{I}_3$ -PEG hybrid material. To gain insight into the underlying photocatalytic mechanism, specific scavenger agents targeting reactive oxygen species (ROS) were introduced, enabling the identification of the primary oxidative species involved in the degradation process. Our findings indicate that more acidic conditions markedly enhance the photocatalytic reduction of Cr(VI), with lower pH values significantly improving the reaction kinetics and overall efficiency. Furthermore, the system demonstrated effective degradation of Cr(VI) at concentrations up to 10 mg/L under controlled irradiation. However, at higher concentrations (between 10 and 20 mg/L), the photocatalytic system exhibited signs of saturation, likely due to limited active sites or increased competition among Cr(VI) and Cr (III) ions, resulting in reduced efficiency.

Among the tested conditions, the nanoroll-dominant sample synthesized at a PEG:Bi molar ratio of 1:1 and a reaction time of 270 min delivered a remarkable 91% reduction of Cr(VI). This outstanding performance underscores the potential of this hybrid nanostructure for practical water purification applications. Overall, these results position  $\text{Bi}_{19}\text{S}_{27}\text{I}_3$ -PEG as a highly efficient, environmentally friendly photocatalyst with significant promise for integration into advanced water treatment technologies aimed at mitigating toxic metal contamination.

---

**KEYWORDS:** Bi 19 S 27 I 3, Photocatalysis, Cr(VI) reduction

---

**ACKNOWLEDGEMENTS:** CSIC I+D Research project "Grupo de Nanomateriales para el Desarrollo Sostenible", PEDECIBA, Heinkel Bentos Pereira and Alvaro Olivera from DDT, CURE, Udelar

### REFERENCES

- [1] L. Ai, L. Wang, N. Guo, M. Xu, D. Jia, C. Tan, X. Jia, W. Cai, Y. Yang, "(Bi 19 S 27 I 3 ) nanorods with more negative potentials of conduction band as highly active photocatalysts under visible light", *Int J Energy Res* 46 (2022) 23857-23870
- [2] M. Mombrú-Frutos, M. Viera, C. Grosso, M. Rodríguez Chialanza, L. Fornaro, M. Eugenia Pérez Barthaburu, I. Aguiar, "Green solution synthesis of Bi 19 S 27 I 3 nanostructures - engineering their morphology through polyethylene glycol and their use in the photocatalytic reduction of Cr(VI)", *J Mater Chem C Mater* (2024) 16843-16853.

## Sputtering as a bottom-up technology for developing Bi-phase structures for efficient green hydrogen production

D. Cavaleiro<sup>1</sup>, J. D. Castro<sup>1</sup>, S. Carvalho<sup>1</sup>, A. Cavaleiro<sup>1, 2 \*</sup>

1) University of Coimbra, Portugal

2) Instituto Pedro Nunes, Coimbra, Portugal

\* albano.cavaleiro AT dem.uc.pt

Green hydrogen has been classified as a vital sustainable solution in relation to energy production and storage [1]. Platinum (Pt) remains the benchmark material for the Hydrogen Evolution Reaction (HER) [2]. However, its high cost and scarcity necessitate the development of cost-effective alternatives, such as transition metal-based phases [3]. If these materials are carefully selected to work in synergy, the electronic and reaction kinetics can be optimised [4]. Moreover, if the electrode morphology is optimised to maximise the active sites the efficiency can be further improved [5]. This work develops bi-phasic thin films based on MoS<sub>2</sub>/Ni with tailored structures to enhance the electrochemically active surface area (ECSA) and reduce HER overpotential. The Ni/MoS<sub>2</sub> thin films were deposited by magnetron sputtering in Ni foam substrates with a multilayered structure. The deposition conditions were selected in order to achieve porous and columnar morphologies. Linear Sweep Voltammetry (LSV) allowed to achieve a current density of 100 mA/cm<sup>2</sup>, with only - 240 mV, and of 400 mA/cm<sup>2</sup>, with only - 315 mV, for the multilayer film, while Ni foam requires - 360 mV and - 395 mV, respectively. ECSA calculations for the multilayer also show almost double the value of that the Ni foam. Chronoamperometry (CA) of the samples in the small scale electrolyser showed an average potential of -363 mV at 100 mA/cm<sup>2</sup> over 24h, much better than the average potential of - 573 mV achieved for the Ni foam.

---

**KEYWORDS:** Multilayer coatings, HER reaction, MoS<sub>2</sub>/Ni biphasic structures, Sputtering, Columnar structures

---

### REFERENCES

- [1] T. Terlouw, C. Bauer, R. McKenna, M. Mazzotti, Large-scale hydrogen production via water electrolysis: a techno-economic and environmental assessment, *Energy & Environmental Science*, 15 (2022) 3583-3602.
- [2] H. Wu, Q. Huang, Y. Shi, J. Chang, S. Lu, Electrocatalytic water splitting: Mechanism and electrocatalyst design, *Nano Research*, 16 (2023) 9142-9157.
- [3] B. Guo, Y. Ding, H. Huo, X. Wen, X. Ren, P. Xu, S. Li, Recent Advances of Transition Metal Basic Salts for Electrocatalytic Oxygen Evolution Reaction and Overall Water Electrolysis, *Nano-Micro Letters*, 15 (2023) 57.
- [4] G. Janani, H. Choi, S. Surendran, U. Sim, Recent advances in rational design of efficient electrocatalyst for full water splitting across all pH conditions, *MRS Bulletin*, 45 (2020) 539-547.
- [5] K. Asha, V.R. Satsangi, R. Shrivastav, R. Kant, S. Dass, Effect of morphology and impact of the electrode/electrolyte interface on the PEC response of Fe<sub>2</sub>O<sub>3</sub> based systems - comparison of two preparation techniques, *RSC Advances*, 10 (2020) 42256-42266.

## Synthesis and cyclic performance of Al<sub>2</sub>O<sub>3</sub>, La<sub>2</sub>O<sub>3</sub>, and MgO stabilized nano CaO sorbents for CO<sub>2</sub> capture

B. Güneş<sup>1</sup>\*, M. Elitaş<sup>1</sup>, H. K. Akben<sup>1</sup>

1) Yeditepe Universtiy, Turkey

\* bayram.gunes AT std.yeditepe.edu.tr

Carbon capture technologies are increasingly important for reducing greenhouse gas emissions in energy-intensive industries such as power generation, cement, iron-steel, and chemical production [1]. Among high-temperature CO<sub>2</sub> sorbents, CaO-based materials are considered highly promising due to their low cost, high theoretical CO<sub>2</sub> uptake capacity, and ease of regeneration during carbonation-calcination cycles [2]. However, pure CaO sorbents suffer from severe sintering, pore collapse, and surface area loss during repeated cycles, leading to rapid performance degradation [3,4].

In this study, four different sorbent systems, namely CaO, CaO-Al<sub>2</sub>O<sub>3</sub>, CaO-Al<sub>2</sub>O<sub>3</sub>-La<sub>2</sub>O<sub>3</sub>, and CaO-Al<sub>2</sub>O<sub>3</sub>-MgO, were synthesized via the sol-gel method in order to improve the cyclic stability and structural durability of CaO-based sorbents. The synthesized materials were characterized using X-ray Diffraction (XRD), Scanning Electron Microscopy coupled with Energy Dispersive Spectroscopy (SEM-EDS), Brunauer-Emmett-Teller (BET) surface area analysis, and Thermogravimetric Analysis (TGA).

XRD analyses confirmed the formation of crystalline CaO phases together with calcium aluminate-related structures that contributed to structural stabilization. SEM observations revealed that the incorporation of Al<sub>2</sub>O<sub>3</sub> improved particle dispersion and reduced agglomeration compared to pure CaO. It was demonstrated by BET analysis that the supported sorbents possessed higher surface area and improved pore accessibility, facilitating gas diffusion during carbonation.

It was observed from TGA cycling experiments that the modified sorbents exhibited significantly improved CO<sub>2</sub> capture stability compared to pure CaO. Among the investigated materials, CaO-Al<sub>2</sub>O<sub>3</sub>-La<sub>2</sub>O<sub>3</sub> demonstrated the highest cycle stability, whereas CaO-Al<sub>2</sub>O<sub>3</sub>-MgO showed enhanced resistance against thermal degradation. The findings indicate that the combined use of support materials and stabilizing additives is an effective strategy for improving the long-term performance of CaO-based sorbents for high-temperature CO<sub>2</sub> capture applications.

---

**KEYWORDS:** Carbon capture, Solid oxide sorbents, Sol-Gel, Calcium loop

---

**ACKNOWLEDGEMENTS:** This work and conference attendance was supported by Yeditepe University.

---

### REFERENCES

- [1] R. Ahmed, G. Liu, B. Yousaf, Q. Abbas, H. Ullah, M. U. Ali, “Recent advances in carbon-based renewable adsorbent for selective carbon dioxide capture and separation - A review”, *Journal of Cleaner Production*, 242, (2020).
- [2] O. Akeeb, L. Wang, W. Xie, R. Davis, M. Alkasrawi, S. Toan, “Post-combustion CO<sub>2</sub> capture via a variety of temperature ranges and material adsorption process: A review”, *Journal of Environmental Management*, 313, (2022).
- [3] B. Arias, M. Alonso and C. Abanades, “CO<sub>2</sub> capture by calcium looping at relevant conditions for cement plants: experimental testing in a 30 kWth pilot plant”, *Industrial & Engineering Chemistry Research*, 56(10), 2634-2640, (2017).
- [4] A. de la Calle Martos, J. M. Valverde, P. E. Sanchez-Jimenez, A. Perejon, C. Garcia-Garrido and L. A. Perez-Maqueda, “Effect of dolomite decomposition under CO<sub>2</sub> on its multicycle CO<sub>2</sub> capture behaviour under calcium looping conditions”, *Physical Chemistry Chemical Physics*, 18(24), 16325-16336, (2016).

## Synthesis and optical properties of CsPbI<sub>3</sub> perovskite films enhanced by Au and Ag plasmonic nanoparticles

S. Mamykin<sup>1\*</sup>, R. Redko<sup>2,3,1</sup>, I. Dmytruk<sup>4</sup>, O. Yeshchenko<sup>4</sup>, N. Berezovska<sup>4</sup>, A. Pinchuk<sup>5</sup>, T. Barlas<sup>1</sup>, V. Romanyuk<sup>1</sup>, N. Romanovska<sup>6</sup>, P. Manoryk<sup>6</sup>

1) V.E. Lashkaryov Institute of Semiconductor Physics, National Academy of Sciences of Ukraine, pr. Nauky 41, 03028, Kyiv, Ukraine, Ukraine

2) V. Lashkaryov Institute of Semiconductor Physics of the National Academy of Sciences of Ukraine, State University of Telecommunications, Ukraine

3) State University of Information and Communication Technologies, Ukraine

4) Taras Shevchenko National University of Kyiv, Ukraine, Ukraine

5) Department of Physics and Energy Science, University of Colorado Colorado Springs, USA

6) L. Pysarzhevskii Institute of Physical Chemistry of the National Academy of Sciences of Ukraine, Ukraine

\* mamykin AT isp.kiev.ua

Cesium-lead-iodide (CsPbI<sub>3</sub>) perovskite thin films have emerged as highly promising materials for next-generation photovoltaic technologies due to their excellent optoelectronic properties. However, reducing the thickness of the perovskite absorber layer to mitigate toxicity and improve environmental stability often leads to reduced light absorption, particularly in the near-infrared (NIR) spectral range where these films are optically thin. To address this trade-off, we report on the synthesis of photosensitive CsPbI<sub>3</sub> thin films integrated with plasmonic metasurfaces comprising Au or Ag nanoparticles of different size and shape. The integration of such plasmonic metal nanostructures into the device architecture is a well-established and highly effective strategy for dramatically enhancing light absorption and carrier dynamics in perovskite solar cells [1].

The plasmonic nanostructures are designed to confine and scatter light at the subwavelength scale by exciting localized surface plasmon resonances (LSPR). In this work, CsPbI<sub>3</sub> films with thicknesses ranging from 100 to 300 nm were synthesized and combined with layers of Au and Ag nanoparticles. The optical constants and structural morphology of the fabricated layers were characterized using multi-angle spectroscopic ellipsometry (SE-2000, Semilab).

Our results demonstrate that placing these plasmonic nanoparticles in close proximity to a metal back-contact supports hybrid "gap modes" [2] which strongly localize the electromagnetic field within the photoactive perovskite layer. While Ag, Au spherical nanoparticles provide substantial absorption enhancement in the visible spectrum, the inclusion of nanorods extends this enhancement into the NIR region. Tuning the inter-particle distance, their size, shape and the composition of the plasmonic layer allows for the precise alignment of the LSPR with the absorption edge of the synthesized CsPbI<sub>3</sub> material [3]. This integrated architecture offers a robust pathway for developing stable, high-performance perovskite solar cells with significantly reduced active layer thicknesses.

---

**KEYWORDS:** Plasmonic metasurfaces, Perovskite solar cells, CsPbI<sub>3</sub>, Au and Ag nanoparticles, Gap modes

---

**ACKNOWLEDGEMENTS:** This work was supported by the NATO SPS project G6197 "Plasmonically Enhanced Perovskite Thin-Film Solar Cells", the National Academy of Sciences of Ukraine within the framework of the project #0125U000799 "New physical principles and technologies for the development of the element base of modern infrared photoelectronics", and the National Research Foundation of Ukraine, project 2025.06/0077 "Technologies for forming passivating coatings for IR photodetectors to increase their detection capability and reliability".

---

### REFERENCES

- [1] Q. Luo, C. Zhang, X. Deng, H. Zhu, Z. Li, Z. Wang, X. Chen, and S. Huang, "Plasmonic effects of metallic nanoparticles on enhancing performance of perovskite solar cells", *ACS Applied Materials & Interfaces*, 9, 34821 (2017).
- [2] D. Y. Lei, A. I. Fernández-Domínguez, Y. Sonnefraud, K. Appavoo, R. F. Haglund Jr, J. B. Pendry, and S. A. Maier, "Revealing plasmonic gap modes in particle-on-film systems using dark-field spectroscopy", *ACS Nano*, 6, 1380 (2012).
- [3] W. Ni, X. Kou, Z. Yang, and J. Wang, "Tailoring longitudinal surface plasmon wavelengths, scattering and absorption cross sections of gold nanorods", *ACS Nano*, 2, 677 (2008).

## Effect of nucleating agents on subcooling and stability of methyl laurate phase change material nanoemulsions

Y. Kim<sup>1</sup>, C. Hermida-Merino<sup>2</sup>, L. Lugo<sup>1</sup>, M. M. Piñeiro<sup>1</sup>, D. Cabaleiro<sup>1</sup> \*

1) *Departamento de Física Aplicada, Universidade de Vigo, E-36310, Vigo, Spain, Spain*

2) *Departamento de Ingeniería Eléctrica, Electrónica, Automática y Física Aplicada, Universidad Politécnica de Madrid, Ronda de Valencia 3, E-28012 Madrid, Spain, Spain*

\* dacabaleiro AT uvigo.es

Phase change material nanoemulsions (PCMEs) are a novel class of thermal fluids developed to simultaneously enhance heat transfer performance and enable latent energy storage functionality [1]. These systems are designed by dispersing submicron-scale droplets of a phase change material within an aqueous carrier fluid [2]. While the formation of finely emulsified droplets is essential for maintaining long-term stability and fluidity, this strategy may also lead to pronounced subcooling of the dispersed phase, which can compromise their thermal effectiveness. As a result, careful optimization of formulation parameters is required to balance dispersion stability and phase transition performance [3].

In this study, PCMEs were formulated using methyl laurate as the phase change material and an ethylene glycol-water mixture as the base fluid. Different dispersed-phase compositions were systematically investigated, including the incorporation of selected *n*-alkanes, fatty alcohols and fatty acids as nucleating agents to enhance colloidal stability and mitigate subcooling effects. The quality of the dispersions was evaluated through dynamic light scattering and zeta potential analyses, confirming good temporal stability of the optimized systems. Differential scanning calorimetry results evidenced that the inclusion of appropriate nucleating agents led to a marked reduction in subcooling, with the methyl laurate/*n*-nonadecane/1-eicosanol combination showing the most favorable phase change characteristics. Additional rheological measurements showed moderate viscosities and mainly Newtonian behavior, supporting the suitability of these nanoemulsions for latent thermal energy storage applications.

---

**KEYWORDS:** Phase change material nanoemulsions, Methyl laurate, Nucleating agents, Subcooling reduction, Transport properties

---

**ACKNOWLEDGEMENTS:** This work was supported by Grant PID2020-112846RB-C21, jointly funded by MCIN/AEI/10.13039/501100011033 and the “ERDF A way of making Europe” Program, as well as by the Xunta de Galicia through the Grant GRC-ED431C 2024/25. C. Hermida-Merino acknowledges financial support from Comunidad de Madrid (Spain) through the “Multiannual Agreement 2023-2026 with Universidad Politécnica de Madrid in, Line A, Emerging PhD researchers” (ref. M230020126A-CNHM). D.C. acknowledges support from the “Research Talent Retention Program for the Year 2025” (University of Vigo, Spain).

---

### REFERENCES

- [1] J. Burgos, R. Mondragón, R. Martínez-Cuenca, U. Nithiyantham, S. Barison, S. Mancin, F. Fabregat-Santiago, and L. Hernández, “Photothermal properties and performance of hybrid carbon-paraffin/water emulsions”, *J. Energy Storage*, 73, 109136 (2023).
- [2] G. Rinaldi, A. Lazaro, M. Delgado, J.M. Marin, and V. Verda, “Use of a low-cost phase change material emulsion in decentralized thermal energy storage for district heating network enlargement”, *Energy*, 306, 132517 (2024).
- [3] D. Cabaleiro, F. Agresti, L. Fedele, S. Barison, C. Hermida-Merino, S. Losada-Barreiro, S. Bobbo, and M.M. Piñeiro, “Review on phase change material emulsions for advanced thermal management: Design, characterization and thermal performance”, *Renew. Sustain. Energy Rev.*, vol. 159, 112238 (2022).

## Solar-activated green synthesis of bio-capped silver nanostructures for environmental and antibacterial applications

S. Alotibi<sup>1\*</sup>

1) Prince Sattam Bin Abdulaziz University, Saudi Arabia

\* sf.alotibi AT psau.edu.sa

This study presents a sustainable solar-activated green synthesis of silver nanostructures using a biomass-derived extract as a dual-function reducing and stabilizing agent. Green synthesis of metal nanoparticles has emerged as a promising alternative to conventional chemical methods due to its environmental compatibility, low cost, and reduced toxicity [1]. Under natural sunlight irradiation, photoactive phytochemicals undergo excitation, generating electrons that facilitate the reduction of  $\text{Ag}^+$  ions into metallic  $\text{Ag}^0$  without the need for external reducing agents or energy-intensive processes [2].

The formation of silver nanostructures was confirmed by a characteristic localized surface plasmon resonance (LSPR) band centered at approximately 450 nm, consistent with previously reported Ag nanoparticle systems [3]. Photoluminescence (PL) analysis revealed significant fluorescence quenching, indicating efficient interfacial electron transfer between excited phytochemicals and the nanoparticle surface [4]. Fourier transform infrared (FTIR) spectroscopy further demonstrated the involvement of oxygen-containing functional groups in both reduction and stabilization processes, confirming the dual role of the biomass extract [5]. Transmission electron microscopy (TEM) analysis showed predominantly spherical nanoparticles with average sizes in the range of 25-35 nm, which is favorable for high surface reactivity and biological interaction [6].

The synthesized nanostructures exhibited strong broad-spectrum antibacterial activity against both Gram-positive and Gram-negative bacteria, in agreement with the well-established antimicrobial properties of silver-based nanomaterials [2],[6]. In contrast, the extract alone showed negligible antibacterial effect, confirming that the activity originates from the formed nanoparticles.

Overall, this work demonstrates an eco-friendly and scalable strategy for the synthesis of functional nanomaterials and provides direct insight into photo-induced reduction mechanisms. The integration of solar energy with waste-derived biomaterials highlights the potential of this approach for environmental remediation and biomedical applications, aligning with emerging sustainable nanotechnology trends [1].

---

**KEYWORDS:** Green synthesis, Silver nanoparticles, Solar-driven processes, Biomass-derived extract, Photoluminescence quenching

---

**ACKNOWLEDGEMENTS:** The authors acknowledge the support of the Applied Physics Laboratory and the University Central Laboratory at Prince Sattam Bin Abdulaziz University for providing access to characterization facilities and technical assistance.

---

### REFERENCES

- [1] J. Singh, T. Dutta, K.-H. Kim, M. Rawat, P. Samddar, P. Kumar, "Green" synthesis of metals and their oxide nanoparticles: applications for environmental remediation. *J. Nanobiotechnol.* 2018, 16, 84.
- [2] H. Rizwana *et al.*, Sunlight-mediated green synthesis of silver nanoparticles using plant extracts and their antibacterial activity. *Molecules* 2022, 27, 2186.
- [3] M. Ider, K. Abderrafi, A. Eddahbi, S. Ouaskit, A. Kassiba, Silver metallic nanoparticles with surface plasmon resonance: synthesis and characterization. *J. Clust. Sci.* 2017, 28, 1051-1069.
- [4] A.M. Queiroz *et al.*, Quenching of fluorescence induced by silver nanoparticles. *Spectrochim. Acta A* 2016, 168, 73-77.
- [5] A. Sati *et al.*, Silver nanoparticles: synthesis, influencing factors and applications. *ACS Omega* 2025, 10, 7549-7582.
- [6] A. Almatroudi, Silver nanoparticles: synthesis, characterization and biomedical applications. *Open Life Sci.* 2020, 15, 819-839.

## Synthesis of starch-based nanoparticles and anthocyanins extracted from ipomoea batatas (L) lam as a potential pH sensor in alkaline media

E. S. Caro<sup>1</sup>\*, J. M. Alejandro<sup>1</sup>, T. Barcellos<sup>2</sup>

1) UTEC, Uruguay

2) UCS, Brazil

\* esmeralda.caro AT utec.edu.uy

Anthocyanins are natural pigments extensively utilized in the food industry due to their potent antioxidant properties and high colorimetric sensitivity to pH variations. While their role as bioactive additives and indicators in food science is well established, research on anthocyanin-based nanoparticles specifically designed as environmental biosolutions remains remarkably scarce. This gap limits the development of sustainable, plant-derived tools for monitoring complex ecological and industrial systems.

Here we demonstrate that biodegradable nanostructures based on native and acetylated starch can successfully encapsulate anthocyanins extracted from *Ipomoea batatas* (L.) Lam, enabling the creation of robust nanostructured environmental sensors. By employing ultrasound-assisted extraction and multi-stage synthesis, we developed formulations that capitalize on the high concentration of stable diacylated peonin and cyanidin derivatives found in this specific sweet potato variety. Our results show that modified starch matrices significantly enhance the stability of these phenolic compounds by reducing aggregation and preserving chromatic intensity. The resulting particulate materials, composed of nanoparticle clusters smaller than 200 nm, exhibit a precise and reproducible colorimetric response across different pH levels. These findings establish that starch-based nanomaterials can successfully overcome the traditional stability barriers of natural pigments while maintaining their functional sensing capabilities.

Spectroscopic analysis using Raman and FTIR techniques allowed the identification of structural and chemical differences among native, gelatinized, and acetylated starch samples, both in the presence and absence of anthocyanins. Acetylation introduced characteristic ester groups, evidenced by the C=O band around  $1735\text{ cm}^{-1}$ , together with a decrease in the intensity of the -OH group. These results confirm the chemical substitution of starch and its improved compatibility with anthocyanins, favoring a more stable encapsulation. In turn, gelatinization caused the disruption of starch crystallinity, facilitating the physical encapsulation of the pigment through the formation of hydrogen bonds. The presence of aromatic bands around  $1600\text{ cm}^{-1}$  and the displacement of the -OH group corroborate the pigment-matrix interaction.

Consequently, this study provides a foundation for the development of sustainable, multifunctional colorimetric systems. Furthermore, these bio-based nanostructures offer a promising pathway for the creation of smart materials and optical sensors for environmental monitoring and agro-industrial applications.

---

**KEYWORDS:** Anthocyanins, Acetylated starch, Nanoencapsulation, Colorimetric response, Environmental pH sensors

---

**ACKNOWLEDGEMENTS:** The authors would like to thank the National Institute for Agricultural Research (INIA) for providing the *Ipomoea batatas* (L.) Lam samples used in this study. We are also deeply grateful to the University of Caxias do Sul (UCS) for providing access to its laboratory facilities and scientific equipment, which were essential for the synthesis and characterization of the starch and anthocyanin-based nanoparticles.

## Controlled synthesis and stability engineering of MAPbX<sub>3</sub> (X = I, Br, Cl) perovskite nanocrystals via e-LARP for multi-functional optoelectronic applications

A. Nath<sup>1\*</sup>, J. R<sup>2</sup>

1) University of Kerala, India

2) Department of Physics, University of Kerala, India

\* adithyanath AT keralauniversity.ac.in

Hybrid organic-inorganic halide perovskite nanocrystals (NCs) have emerged as intriguing materials for next-generation optoelectronic devices due to their tunable bandgaps, high absorption coefficients, and superior emission properties. Low-cost and scalable fabrication is further made possible by their solution processability [1]. Despite these benefits, MAPbX<sub>3</sub> (X = I, Br, Cl) nanocrystals environmental sensitivity and structural phase instability severely restrict their usefulness. Specifically, halide content has a significant impact on optical response, degradation routes, and crystal symmetry, which calls for a comprehensive understanding of composition-dependent behavior [2]. Although stability-performance trade-offs are still unsolved, recent developments in colloidal synthesis have enhanced optical performance [3]. Here, we tackle the problem of retaining device-level functionality while attaining regulated synthesis and stability throughout the entire MAPbX<sub>3</sub> halide series. We show that composition-dependent adjustment of structure, stability, and optoelectronic performance in MAPbX<sub>3</sub> nanocrystals is possible using a modified emulsion-assisted ligand-assisted reprecipitation (E-LARP) approach [4]. Glovebox-assisted MAPbI<sub>3</sub> NCs have a tetragonal phase (I<sub>4</sub>/mcm) with a direct bandgap of around 1.55 eV and a strong absorption edge at 770-780 nm. However, they rapidly degrade under ambient circumstances due to hydrate formation and deprotonation, which results in considerable electrical deterioration. On the other hand, glovebox-free synthesized MAPbBr<sub>3</sub> NCs form highly crystalline cubic structures with preferential (040) and (113) orientations, exhibiting narrow linewidth, improved carrier lifetimes, and intense green emission (~532 nm), resulting in device performance with a fill factor of 43.56% and a Voc of 0.67 V. Additionally, MAPbCl<sub>3</sub> NCs produced in ambient environments show improved stability, a broad bandgap (~3 eV), a high photoluminescence quantum yield (68.9%), and quick carrier dynamics, allowing for photodetectors with detectivity of  $1.12 \times 10^9$  Jones. These results demonstrate the versatility of MAPbX<sub>3</sub> nanocrystals for photovoltaic, light-emitting, and photodetection applications and demonstrate a clear correlation between composition, structure, property, and stability. In addition to offering crucial insights for creating stable perovskite nanoparticles for multifunctional optoelectronic systems, this work offers a scalable synthesis strategy.

**KEYWORDS:** Halide perovskite nanocrystals, MAPbX<sub>3</sub> (X = I, Br, Cl), Emulsion ligand-assisted reprecipitation (e-LARP), Stability engineering, Optoelectronic applications

**ACKNOWLEDGEMENTS:** Author would like to thank the University of Kerala, Thiruvananthapuram, for providing financial assistance under the JRF/SRF scheme.

### REFERENCES

- [1] N. Zhang, Q. Na, Q. Xie, and S. Jia, “Development of Solution-Processed Perovskite Semiconductors Lasers,” *Crystals* (Basel), vol. 12, no. 9, p. 1274, Sep. 2022, doi: 10.3390/cryst12091274.
- [2] T. A. Berhe *et al.*, “Organometal halide perovskite solar cells: degradation and stability,” *Energy Environ. Sci.*, vol. 9, no. 2, pp. 323-356, 2016, doi: 10.1039/C5EE02733K.
- [3] H. Huang *et al.*, “Emulsion Synthesis of Size-Tunable CH<sub>3</sub>NH<sub>3</sub>PbBr<sub>3</sub> Quantum Dots: An Alternative Route toward Efficient Light-Emitting Diodes,” *ACS Appl. Mater. Interfaces*, vol. 7, no. 51, pp. 28128-28133, Dec. 2015, doi: 10.1021/acsami.5b10373.
- [4] A. N. R. A. Raj, and R. Jayakrishnan, “Emulsion-LARP method: Optimization of demulsifier for synthesis of methylammonium lead bromide nano-structures,” *Nanoscale*, vol. 17, no. 33, pp. 19344-19352, 2025, doi: 10.1039/D5NR01718A.

## Nanocomposite zeolite-based adsorbents for selective removal of cesium radionuclides from contaminated waters

Y. Bondar<sup>1\*</sup>, S. Kuzenko<sup>2</sup>, K. Yaroshenko<sup>3,2</sup>

1) Czech University of Life Sciences Prague, Kamýcká 129, 165 00, Prague - Suchbát, Czech Republic, Czech Republic

2) State Institution “the Institute of Environmental Geochemistry of National Academy of Sciences of Ukraine”, Ukraine

3) Institute of Geological Sciences of National Academy of Science of Ukraine, Ukraine

\* juliavad AT yahoo.com

The development of efficient and selective adsorbents for radionuclide removal from contaminated water is essential for minimizing hazardous liquid radioactive waste and improving the safety of radioactive waste management. Natural zeolites have long been applied for cesium radionuclides removal due to their ion-exchange properties, low cost, and environmental compatibility. However, their adsorption efficiency decreases in highly mineralized solutions because of reduced selectivity in the presence of competing alkali metal ions, as well as the partially reversible nature of cesium adsorption.

Transition metal ferrocyanides are considered one of the most effective highly selective adsorption materials for cesium ions. However, their practical application in aqueous systems is limited by the formation of fine powders with poor colloidal stability, as well as by the difficulties associated with separating spent adsorbent. For this reason, developing composite zeolite-based adsorbents with incorporated ferrocyanide phase is a promising approach. This combines the mechanical stability, permeability and low cost of zeolites with the high cesium selectivity of ferrocyanides.

In this study, a composite adsorbent for selective removal of cesium radionuclides was synthesized by incorporating a potassium-copper ferrocyanide phase to the zeolite matrix. Structural and morphological characterization by scanning electron microscopy, X-ray diffraction, and Fourier-transform infrared spectroscopy confirmed the successful formation of a ferrocyanide phase consisting of uniformly distributed rounded nanoparticles on the zeolite surface.

The adsorption properties of natural and composite zeolite granules (1-2 mm) were investigated in single- and multicomponent model solutions with elevated concentrations of competing ions. The results demonstrated that solution mineralization had a strong effect on cesium uptake by natural clinoptilolite, whereas the composite adsorbent retained high adsorption efficiency and selectivity under high-salinity conditions. Furthermore, incorporating the potassium-copper ferrocyanide phase enhanced the stability of immobilized cesium and reduced the reversibility of adsorption. This indicates the potential applicability of the developed composite material in the treatment of radioactive liquid waste and contaminated waters.

---

**KEYWORDS:** Nanocomposite adsorbent, Ferrocyanide nanoparticles, Zeolite, Cesium radionuclides, Liquid radioactive waste

## Unlocking the photocatalytic potential of semiconductor metal oxides using octahedral molybdenum clusters

M. Dubovsky<sup>1\*</sup>, K. Kirakci<sup>1</sup>, G. T. Karthikeyan<sup>1</sup>, M. Stastny<sup>1</sup>, J. Henych<sup>1</sup>

*1) Institute of Inorganic Chemistry, Czech Academy of Sciences, Czech Republic*

\* dubovsky AT iic.cas.cz

Several metal oxide-based materials, such as nanostructured titania ( $TiO_2$ ) or ceria ( $CeO_2$ ), have been established as materials potentially suitable for the remediation of contaminated waters.

One of the reasons for their applicability is their properties as photocatalysts, functioning as such due to their unique structural (e.g., abundance of surface hydroxyl groups, structural defects) and physical/electronic (e.g., sufficient band gap width) features. [1,2]

However, real world applications of these materials still face several issues, mainly due to their insufficient ability to absorb visible light, leading to their use primarily under UV light irradiation, making their real world use economically and practically difficult. [3]

This research deals with the modifications of metal oxide photocatalysts using octahedral molybdenum clusters, which are phosphorescent dyes with excellent visible light absorption properties, and the ability to produce reactive oxygen species, mainly singlet oxygen. [4] Composites, using titania and ceria, with a variety of different molybdenum clusters were prepared using simple and cheap synthesis methods, ensuring fast and highly reproducible fabrication process.

The composites were tested on model phenolic compounds (phenol, BPA, BPS), as well as microplastics. They exhibit superior ability to remove and decompose pollutants in water under visible light irradiation, owing to dye sensitization, which promotes efficient energy transfer and prolonged electron-hole separation. Synergistic functionality between several produced reactive oxygen species (hydroxyl radicals and singlet oxygen), is also shown to play a significant role. The results presented demonstrate that cluster-modified metal oxides offer a highly efficient, sustainable pathway for solar-driven wastewater remediation, moving advanced photocatalysis closer to viable large-scale environmental applications.

---

**KEYWORDS:** Titania, Nanoceria, Molybdenum clusters, Photocatalysis, Dye sensitization

---

**ACKNOWLEDGEMENTS:** Projects no. UJEP-IGA-2026-53-005-2 ( $CeO_2$ /Metal Carbides Hybrid Nanostructures for Advanced Functional Materials), funded by UJEP Internal Grant Agency, and no. UJEP-SGS-2025-44-003-2 (Photoactive Nanocomposite Materials Based on Molybdenum Clusters and Functional Nanoparticles), funded by UJEP Student's Grant Competition, as well as the international joint initiative EIG Concert Japan, are all gratefully acknowledged.

---

### REFERENCES

- [1] M. Šťastný, D. Bovol, J. Tolasz, P. Bezdička, J. Čundrle, M. Kormunda, I. Dimitrov, P. Janoš, K. Kirakci, and J. Henych, "Interfacial behavior of ceria grown on graphene oxide and its use for hydrolytic and photocatalytic decomposition of bisphenols A, S, and F", *Environ. Sci. Nano.* 12, 502-513 (2025).
- [2] G. Issa, S. Křížnecká, P. Bezdička, D. Popelková, M. Kormunda, J. Ederer, D. Bůžek, J. Čundrle, Z. Baďura, J. Henych and M. Šťastný, "Dual-mode catalytic degradation of diclofenac by copper oxide-modified  $TiO_2/MnO_x$  composites: insights from dark and UV-A activation", *Catalysis Science and Technology* 15(15), 4438-4456 (2025)
- [3] X. Liu, Y. Chen, Y. Tao, L. Shen, Z. Xu, Z. Bian, H. Li, "Challenges of photocatalysis and their coping strategies", *Chem Catalysis* 2(6), 1315-1345 (2022)
- [4] K. Kirakci, M. A. Shestopalov, and K. Lang, "Recent developments on luminescent octahedral transition metal cluster complexes towards biological applications", *Coordination Chemistry Reviews* 481 (2023)

## Multifunctional composite including inorganic nanoparticles for modifying polymer microporous filtration membrane

Ponomarova<sup>1\*</sup>, L. Rozhdesvenska<sup>2</sup>, V. Chmilenko<sup>2</sup>, K. Kudelko<sup>2</sup>, V. Ushkalov<sup>3</sup>, L. Vygovska<sup>3</sup>, A. Palchik<sup>2</sup>, O. Tymoshenko<sup>4</sup>

1) Sumy State University, Ukraine

2) V. Vernadsky Institute of General and Inorganic Chemistry, NAS of Ukraine, Ukraine

3) National University of Life and Environmental Sciences of Ukraine, Ukraine

4) Igor Sikorsky National Technical University of Ukraine, Ukraine

\* l.ponomarova AT chem.sumdu.edu.ua

The performance of commercial polymer membranes: for microfiltration and ultrafiltration of the liquids of technical and biological origin is complicated by low permeate flux down to the stop of filtration process, and by long-time regeneration of the membrane systems, which requires a considerable amount of reagents and pure water for rinsing. These problems are caused by low hydrophilicity of commercial membranes made of PVDF, PES, ePTFE, since organic substances and microorganisms adhere to hydrophobic material causing its fouling. Polymer membranes to foul can be overcome by their modifying with inorganic nanoparticles - they perform hydrophilizing function so far as hydration shells around them prevent undesirable adhesion. Main approaches: (i) blending the solution of polymer with preliminarily synthesized inorganic nanoparticles followed by the membrane formation, (ii) attaching preliminarily synthesized nanoparticles to the surface of preliminarily formed membrane or their embedding into pores, (iii) synthesis of nanoparticles on the surface of preliminarily formed membrane or inside its pores (for commercial membranes, the directions (ii) and (iii) are suitable). Modifying asymmetric membranes containing active layer allows one not only to prevent fouling, but also to ensure the separation ability towards one or other species. There is a problem for symmetric macroporous membranes to fill pores as much as possible in order to provide retention of colloidal species. In this work, we modified macroporous ePTFE membranes with a composite containing polymer (filling pores), nanoparticles of zirconium hydrophosphate (hydrophilizing, enhancement of mechanical durability), silver nanoparticles, (bactericidal activity), advanced carbon nanomaterials (hydrophilizing, enhancement of AgNPs activity), the combinations of directions (ii) and (iii) were used. To facilitate modifying, the membranes were preliminarily treated with synthetic (polyethyleneimine, acetylacetonate zirconium complex) and natural agents (collagen, polysaccharides, particularly with those generated by bacteria), as a result, the water contact angle decreased from  $>90^\circ$  down to  $20^\circ$ . The membranes demonstrate cut-off against bovine serum albumin, ovalbumine and lactalbumine indicating the pore size of  $<10$  nm. The modified membranes show the flux recovery ratio of 50%, the permeability of  $\approx 100$  L m<sup>-2</sup>h<sup>-1</sup>bar<sup>-1</sup>. It was found the transformation of microfiltration membranes into ultrafiltration materials as well as their stability against fouling and biofouling. The membranes can be applied to the production of multichannel tubular modules, where more massive and fragile ceramic membranes are usually used. The membranes are recommended for water and wastewater treatment as well as for needs of food industry and nanotechnologies. Further development of the work can be directed to the membrane application for the treatments of various solutions of natural, technogenic and biogenic origin.

**KEYWORDS:** EPTFE membranes, Zirconium hydrophosphate, Silver nanoparticles, Surface modification, Biofouling resistance

**ACKNOWLEDGEMENTS:** The work was performed within the framework of program No. 0126U000968 entitled "Development of a reactor based on bioactive organo-inorganic composites and membranes for the neutralization of toxic compounds in aqueous solutions and wastewater." The program was supported by the National Academy of Sciences of Ukraine.

## Tribological evaluation of dynamic friction and durability of resin nanostructured surfaces

H. Kawashima<sup>1</sup>\*

*1) Kansai University, Japan*

\* k083756 AT kansai-u.ac.jp

Nanostructures on cicada wings exhibit bactericidal properties [1]; however, their tribological behavior and durability remain unclear [2]. In this study, resin nanostructured surfaces with nanopillar geometries were fabricated by thermal nanoimprint lithography using anodic aluminum oxide (AAO) templates. The dynamic friction coefficient was evaluated under repeated unidirectional sliding (up to 1000 cycles) with varying normal loads, and structural changes after testing were examined by scanning electron microscopy (SEM).

The friction coefficient increased rapidly in the initial stage (0-50 cycles), followed by a gradual increase, regardless of nanostructure shape and height, indicating that the initial increase is governed by changes in contact conditions. Although some nanostructured surfaces exhibited lower friction coefficient than that on a flat surface under certain conditions, no consistent dependence on geometry was observed [3]. SEM observations revealed tip deformation without significant fracture, indicating sufficient durability.

These results demonstrate that friction behavior is governed more by contact conditions and deformation than by nanostructure geometry.

---

**KEYWORDS:** Nanostructured surface, Dynamic friction coefficient, Tribology

---

**ACKNOWLEDGEMENTS:** This research was conducted in part using the ORDIST HRC cleanroom at Kansai University.

---

### REFERENCES

- [1] E.P. Ivanova *et al.*, *Small* 8 (2012) 489-2494.
- [2] M.I. Ishak *et al.*, *J. Colloid Interface Sci.*, vol. 583, pp. 414-424, 2021.
- [3] Q. Cui *et al.*, *ACS Appl. Nano Mater.*, vol. 3, pp. 4599-4609, 2020.

## The influence of finishing chemical treatment on the formation of a nanostructured surface of InSb substrates

G. Malanych<sup>1</sup>\*

1) V.E. Lashkaryov Institute of Semiconductor Physics, National Academy of Sciences of Ukraine, pr. Nauky 41, 03028, Kyiv, Ukraine, Ukraine

\* galya.malanich AT gmail.com

Indium antimonide InSb is an important narrow bandgap semiconductor for infrared optoelectronic devices, high sensitivity sensors, and related electronic applications. The performance and reproducibility of InSb based devices depend strongly on the quality of substrate surface preparation. Surface defects, residual damage, crystallographic anisotropy, and insufficient control of the final polishing stage can limit device fabrication and degrade functional properties. Therefore, controlled chemical treatment of InSb substrates remains an important technological problem.

This work investigates the influence of finishing chemical treatment on the formation of ultra smooth InSb surfaces with different crystallographic orientations. Particular attention is given to iodine containing etching compositions based on I<sub>2</sub> and HI. These solutions are considered as an alternative to I<sub>2</sub> based methanol etchants because they provide stable polishing behavior, long storage stability, and improved process controllability. Chemical dynamic polishing and chemical mechanical polishing were compared as finishing treatments for InSb substrates with (111)A, (111)B, (110), (100), and (211) orientations.

It was found that I<sub>2</sub> and HI etching compositions produce a polishing effect on all investigated InSb orientations. Atomic force microscopy showed that chemical dynamic polishing is suitable as the final treatment stage for InSb (111), (110), and (100) substrates, whereas chemical mechanical polishing is more effective for substrates with (211) orientation. The minimum polishing rate was obtained for an etching mixture containing 3 mass.% iodine, which enabled controlled and uniform material removal. Depending on crystallographic orientation, the arithmetic average roughness Ra after finishing treatment was in the range of 0.43 to 1.06 nm.

The results show that optimized I<sub>2</sub> and HI based finishing treatment enables uniform removal of thin damaged surface layers and formation of mirror like InSb surfaces with controlled nanorelief. Such surface preparation is important for the fabrication of next generation InSb optoelectronic and infrared sensor devices.

---

**KEYWORDS:** Ultra-smooth surface, Crystallographic orientation, Indium antimonide (InSb), Chemical polishing

---

**ACKNOWLEDGEMENTS:** This work was supported by the National Academy of Sciences of Ukraine (Project No. III-10-24). The authors express their sincere gratitude to the defenders of Ukraine and the personnel of the Ministry of Emergency Situations, whose courage and dedication made it possible to carry out this research and share the results with the scientific community.

## Performance evaluation of TiO<sub>2</sub>-water nanofluid in nuclear power plant spent fuel pool heat exchangers

T. Rymar<sup>1</sup>, A. Leshchov<sup>1</sup> \*

1) Lviv Polytechnic National University, Ukraine

\* artem.leshchov.ae.2023 AT lpnu.ua

Ensuring an efficient and stable heat exchange process of nuclear power plant (NPP) systems is a critical aspect of safety during NPP operations. To improve it, it is proposed to use TiO<sub>2</sub> nanofluid as a heat carrier in spent fuel pool heat exchangers TG(11-13)W<sub>01</sub>. Adding nanoparticles to the base fluid enhances its thermal properties, but increases viscosity, therefore increasing hydraulic resistance and required pumping power. This work investigates the expediency of using TiO<sub>2</sub>-water nanofluid in TG(11-13)W<sub>01</sub> heat exchangers by comparing specific pump power as a function of the heat transfer coefficient ( $N(\alpha)$ ) for different TiO<sub>2</sub> volume fractions ( $\varphi$ ).

The thermophysical properties of nanofluid were calculated for nanoparticle volume fraction ranging from 0.2% to 0.8%, and velocities 1.5 - 2.1 m/s, with maximum heat exchanger operating temperature of 70 °C. The dimensions of the heat exchanger under study were adopted from operating typical prototypes. The properties of base fluid and nanoparticles were calculated using data fitting curves proposed in the following references [1, 2], the nanofluid properties were calculated as proposed [1, 3, 4]. The Nusselt number of nanofluid was calculated using B. S. Petukhov's equation [5].

The results show an increase of the heat transfer coefficient on the whole studied range of volume fraction and velocity, with a peak at  $\varphi = 0.6\%$ . However, by comparing  $N(\alpha)$  curves, it was found that the most efficient volume fraction considering pressure losses due to increased viscosity, is  $\varphi = 0.4\%$ . The results of this theoretical research can be used to intensify heat exchange efficiency in operating NPP spent fuel pool heat exchangers without significant design changes, or decrease required pumping power and electricity usage, while maintaining same heat exchange rate. All the modifications must take the increased price of heat exchange nanofluid into consideration.

---

**KEYWORDS:** Heat transfer nanofluids, Nuclear spent fuel pool heat exchanger, TG11W01 heat exchanger, TiO<sub>2</sub>, Heat transfer enhancement

---

### REFERENCES

- [1] A. A. Abbasian Arani and J. Amani, "Experimental study on the effect of TiO<sub>2</sub>-water nanofluid on heat transfer and pressure drop," *Experimental Thermal and Fluid Science*, vol. 42, pp. 107-115, Oct. 2012, doi: 10.1016/j.expthermflusci.2012.04.017.
- [2] P. J. Linstrom and W. G. Mallard, Eds., "Anatase (TiO<sub>2</sub>)," in *NIST Chemistry WebBook*, NIST Standard Reference Database Number 69, National Institute of Standards and Technology, Gaithersburg, MD. [Online]. Available: <https://webbook.nist.gov>.
- [3] B. K. Dandoutiya and A. Kumar, "Comparison of Mathematical Models to Estimate the Thermal Conductivity of TiO<sub>2</sub>-Water Based Nanofluid: A Review," *Thermal Science*, vol. 26, no. 1B, pp. 579-591, 2022, doi: 10.2298/TSCI201026224D.
- [4] M.K. Meybodi *et al.*, A novel correlation approach for viscosity prediction of water based nanofluids of Al<sub>2</sub>O<sub>3</sub>, TiO<sub>2</sub>, SiO<sub>2</sub> and CuO, *Journal of the Taiwan Institute of Chemical Engineers* (2015), <http://dx.doi.org/10.1016/j.jtice.2015.05.032>.
- [5] B.S. Petukhov, Heat transfer and friction in turbulent pipe flow with variable physical properties, in: T.F. Irvine, J.P. Hartnett Jr. (Eds.), *Advances in Heat Transfer*, vol. 6, Academic Press, Inc., New York, 1970, pp. 504-564.

## Nanostructured montmorillonite-based sorbents for uranium removal: Role of activation sequence and surface modification

I. Kovalchuk<sup>1</sup> \*

*1) Institute for Sorption and Problems of Endoecology, Ukraine*

\* kovalchukiryna AT gmail.com

Nanoscale architecture of layered clay minerals provides a versatile platform for tuning surface properties and functional performance in environmental applications. In montmorillonite-based systems, the sequence of chemical and physicochemical treatments governs the modification of native layer organization, defect density, and interlayer accessibility, which ultimately control sorption behavior toward uranium species.

This study presents a comparative analysis of uranium sorption by montmorillonite subjected to two distinct modification routes: (i) acid activation followed by surfactant modification, and (ii) surfactant-modified montmorillonite subsequently treated by mechanical activation. Although both approaches involve chemical and physicochemical transformations of the clay structure, they generate fundamentally different surface states and sorption environments.

The first approach, involving acid activation followed by surfactant functionalization, produced a material with enhanced surface area and a transition from cation-exchange behavior to effective uptake of anionic and neutral uranium species. This system exhibited stable performance under highly mineralized water conditions (up to 12 g/L), with sorption well described by a Langmuir-type mechanism indicating relatively uniform active sites.

In contrast, the second approach, based on high-energy mechanochemical activation of organo-modified montmorillonite, resulted in pronounced structural disorder, delamination, and defect generation, while preserving surfactant-induced surface functionality. This synergistic combination led to a substantial increase in sorption performance, reaching nearly an order of magnitude higher uranium uptake. This reflects the formation of energetically heterogeneous adsorption sites governed by both surface complexation and electrostatic interactions. Sorption in this case was best described by Freundlich and Temkin models, confirming a multi-site and energetically diverse adsorption system.

The results demonstrate that treatment sequence-controlled nanostructuring of montmorillonite enables targeted tuning of uranium sorption mechanisms. This approach provides a flexible platform for designing clay-based nanomaterials for reactive barriers, water treatment systems, and engineered environmental protection technologies.

---

**KEYWORDS:** Layered nanomaterials, Treatment sequence, Sorption mechanisms, Surface defects, Uranium removal

## Carrier recombination in inorganic CsPbI<sub>3</sub> perovskite nanocrystals

S. Mamykin<sup>1</sup>, R. Redko<sup>2, 3, 1\*</sup>, I. Dmytruk<sup>4</sup>, O. Yeshchenko<sup>4</sup>, N. Berezovska<sup>4</sup>, A. Pinchuk<sup>5</sup>, N. Romanovska<sup>6</sup>, P. Manoryk<sup>6</sup>

1) V.E. Lashkaryov Institute of Semiconductor Physics, National Academy of Sciences of Ukraine, pr. Nauky 41, 03028, Kyiv, Ukraine, Ukraine

2) V. Lashkaryov Institute of Semiconductor Physics of the National Academy of Sciences of Ukraine, State University of Telecommunications, Ukraine

3) State University of Information and Communication Technologies, Ukraine

4) Taras Shevchenko National University of Kyiv, Ukraine, Ukraine

5) Department of Physics and Energy Science, University of Colorado Colorado Springs, USA

6) L. Pysarzhevskii Institute of Physical Chemistry of the National Academy of Sciences of Ukraine, Ukraine

\* redko.rom AT gmail.com

All-inorganic CsPbX<sub>3</sub> (X=Cl, Br, I) perovskites have emerged as a compelling solution to well-known stability problem. By replacing the organic cation with cesium Cs<sup>+</sup>, CsPbI<sub>3</sub> provides an inorganic lattice framework that is significantly more robust against thermal degradation. Moreover, with a bandgap of ~1.73-1.80 eV, CsPbI<sub>3</sub> possesses a near-ideal bandgap for tandem solar cell configurations (as the top layer) and for intermediate-band photovoltaics.

CsPbI<sub>3</sub> nanostructures were synthesized using a modified hot-injection method, which is known for producing high-quality and size-monodisperse all-inorganic nanocrystals. Cesium oleate, prepared by dissolving cesium carbonate Cs<sub>2</sub>CO<sub>3</sub> in cyclohexanone and oleic acid, and lead iodide PbI<sub>2</sub>, dissolved in octadecene with oleic acid and oleylamine under vacuum and heated at 120°C, were the precursors. The PbI<sub>2</sub> precursor was heated to 160°C under argon before the cesium oleate was rapidly injected. The solution was immediately quenched in an ice bath to stop growth. The resulting nanocrystals were purified by several cycles of centrifugation in cyclohexane, and finally dispersed in cyclohexane.

Optical measurements were carried out at room temperature (295 K) in an ambient atmosphere using a FS<sub>5</sub>-SS v2 Spectrophotometer. The emission was collected at 700 nm and detected by a single photon counting photomultiplier in temperature stabilised housing (PTM-980).

Our steady-state room temperature PL and PLE results reveal a narrow emission peak centered at 1.77 eV, which is nearly resonant with the band-edge absorption. The extremely small Stokes shift observed (<10 meV) is indicative of the small number of trap states in band gap energy region. This high spectral purity, combined with a Full Width at Half Maximum (FWHM) of less than 35 nm, positions CsPbI<sub>3</sub> as an exceptional material for high-definition light-emitting diodes (LEDs) and efficient intermediate-band solar cells. Furthermore, time-resolved photoluminescence (TRPL) measurements demonstrate a multi-exponential decay profile over a large temporal range. We interpret these dynamics through a rigorous tri-exponential recombination model, extracting individual lifetime components ( $\tau_1=83.2$  ns,  $\tau_2=257.2$  ns, and  $\tau_3=674.2$  ns). These components collectively suggest a high crystalline quality with effective suppression of surface defects and long-lived carrier states, supporting high efficiencies.

Obtained results demonstrate that the fully inorganic CsPbI<sub>3</sub> framework can deliver exceptional optoelectronic performance. The remaining challenge now is practical phase-stabilization of the active black  $\alpha$ -phase, as well as the optimization of thin-film processing, to translate these high material-level efficiencies into robust, stable, and high-performance devices. Future research should prioritize advanced passivation techniques to further suppress the surface defect-related decay component ( $\tau_1$ ) and enhance the longevity of the active phase

---

**KEYWORDS:** Perovskites, Photovoltaics, Nanocrystals, Photoluminescence

---

**ACKNOWLEDGEMENTS:** This work was supported by the NATO SPS project G6197 “Plasmonically Enhanced Perovskite Thin-Film Solar Cells”, and the National Academy of Sciences of Ukraine (project No. 4.11/23-P)

## Development of regeneration methods for heterostructured photocatalysts in CO<sub>2</sub> gas-phase reduction systems

D. Gavars<sup>1</sup>\*, A. Felsharuk<sup>1</sup>, D. Erts<sup>1</sup>, J. Andzane<sup>1, 1</sup>

1) University of Latvia, Institute of Chemical Physics, Latvia

\* davis.gavars AT lu.lv

Global climate change is an escalating issue driven by the accumulation of atmospheric greenhouse gases, which calls for an urgent transition toward sustainable carbon management [1]. One of the main aspects of this is the mitigation of CO<sub>2</sub> emissions, which requires innovative technologies capable of converting the highly stable CO<sub>2</sub> molecule into higher-value chemical compounds, such as methanol and formic acid [2]. Photocatalysis has been presented as a particularly promising strategy, using solar energy to facilitate catalytic CO<sub>2</sub> reduction under ambient conditions. However, the long-term industrial viability of these catalysts is often impeded by rapid deactivation and diminishing efficiency over time. Addressing these limitations through effective photocatalyst regeneration is therefore critical to maintaining high catalytic performance and ensuring the economic feasibility of solar-to-fuel conversion technologies.

Previously, our group has utilized different nanostructured heterostructures fabricated from metal oxides, chalcogenides, and carbon nanotubes for photocatalytic CO<sub>2</sub> reduction. Contrary to most research, where photocatalysis is realized through a liquid medium, our work has been focused on the photocatalytic processes occurring in the gas phase [3]. The main reason for photocatalyst decay in gas-phase systems is the progressive contamination of the material surface, often resulting from the strong adsorption of carbon-based intermediates or the accumulation of carbon buildup [4]. These side products block active sites and prevent the catalyst from absorbing incoming light, which in turn lowers efficiency. To counteract this, several reactivation strategies are employed, such as thermal oxidation, solvent extraction, or photo-oxidative cleaning to break down contaminants using light or UV irradiation.

While thermal oxidation is highly effective and fast, higher temperatures risk destroying sensitive nanostructures and inducing phase changes [5]. Similarly, photo-oxidative cleaning offers a convenient approach but is often limited by slow reaction rates and an inability to remove deeply embedded or non-reactive residues. Solvent washing is gentle but requires a tedious drying process and risks potential structural collapse due to capillary forces. For solid photocatalysts in the gas phase, low-temperature thermal oxidation is the easiest method and could generally prove most effective, as it allows for the complete removal of contaminants without the structural damage or extra waste associated with chemical washing.

This study examines the optimization of thermal oxidation as the main regeneration method, balancing the need for complete surface cleaning with the preservation of catalyst morphology. By exploring these potential recovery conditions, this research aims to provide a more practical strategy for maintaining the long-term performance and durability of solid-state photocatalysts in gas-phase environments.

---

**KEYWORDS:** Photocatalyst regeneration, CO<sub>2</sub> Reduction, Nanostructured photocatalysts, Metal oxides

---

**ACKNOWLEDGEMENTS:** Project No. 1.1.1.8/1/24/I/003 "Strengthening the Research and Development Capacity of Doctoral Studies at the University of Latvia in the Fields of Smart Specialisation"

---

### REFERENCES

- [1] A. Mufeedah Muringa Kandy, Rajeev, and M. Sankaralingam. "Development of proficient photocatalytic systems for enhanced photocatalytic reduction of carbon dioxide." *Sustainable Energy & Fuels* 5, 1, 12-33 (2021).
- [2] G. Guangfu Liao, B. Ding, Yang, and C. Li. "Challenges in photocatalytic carbon dioxide reduction." *Precision Chemistry* 2, 2, 49-56 (2024).
- [3] M. Schreck, and M. Niederberger. "Photocatalytic gas phase reactions." *Chemistry of Materials* 31, 3, 597-618 (2019).
- [4] Y. Xiaojun Yan, C. Tang, Y. Ma, Liu, and J. Xu. "Deactivation and regeneration of photocatalysts: A review." *Desalination and Water Treatment* 124, 160-176 (2018).
- [5] M. Chao Zhang, Z. Tao, N. Sui, Y. An, Shen, and X. Zhou. "Influence of oxidation temperature on the regeneration of a commercial Pt-Sn/Al<sub>2</sub>O<sub>3</sub> propane dehydrogenation catalyst." *Catalysts* 14, 6, 389 (2024).

## Boosting the durability and activity of platinum-based cathode catalysts for pem fuel cells: The role of cerium and cobalt doping on graphene oxide support

A. Marinoiu<sup>1\*</sup>, I. Vagner<sup>1</sup>, S. Pintilie<sup>1</sup>, M. Varlam<sup>2</sup>

1) Institute for Cryogenics and Isotopic Technologies - ICSI, Ramnicu Valcea, Romania, Romania

2) Institute for Cryogenics and Isotopic Technologies - ICSI, Rm Valcea, Romania

\* adriana.marinoiu AT icsi.ro

The transition towards a sustainable hydrogen economy involves the development of highly efficient and durable electrocatalysts for Proton Exchange Membrane Fuel Cells (PEMFC). Since platinum (Pt) still remains the commercial catalyst, its high cost and susceptibility to degradation under acid specific operating conditions in PEMFC limit large-scale commercialization. This study investigates a series of mono-, bi-, and trimetallic nanocatalysts (Pt-Co, Pt-Ce, and Pt-Co-Ce) anchored on Graphene Oxide (GO) supports, synthesized via a controlled microwave chemical route. The doping of Cobalt (Co) and Cerium (Ce) aims to modulate the electronic structure of Pt and enhance the catalyst's durability. Cerium, through its  $Ce_3^+/Ce_4^+$  redox oxygen storage capacity, acts as a sacrificial agent against oxidative stress, while Cobalt promotes the compressive strain on Pt lattices, optimizing the Oxygen Reduction Reaction (ORR) kinetics.

The samples were characterized by TEM, BET and TGA, and the electrochemical performance was evaluated by cyclic voltammetry (CV), linear sweep voltammetry (LSV) and chronoamperometry (CA). The obtained results indicate that the trimetallic Pt-Co-Ce/rGO electrocatalyst exhibits improved electrochemical activity and superior stability for the oxygen reduction reaction (ORR), compared to monometallic and bimetallic materials. In addition, electrocatalysts were also evaluated for the hydrogen evolution reaction (HER), the results indicating that all samples have HER activity and good short-term electrochemical stability under the applied test conditions.

These results highlight the potential of modifying Pt/rGO by controlled introduction of Co and Ce as an effective strategy for improving electrocatalytic activity and stability, contributing to the development of Pt-based materials with superior performance for electrochemical energy conversion applications.

---

**KEYWORDS:** PEM fuel cells, Pt-based catalysts, Graphene oxide support, Cerium and cobalt doping

---

**ACKNOWLEDGEMENTS:** This work was supported by the project PN 23 15 01 03, Contract No. 20N/2023, Core Program within the National Research Development and Innovation Plan 2022-2027, financed by Ministry of Research, Innovation, Digitization of Romania and by the project RO-HydroHub "Romanian Hydrogen and New Energy Technologies Hub", contract nr. G2025-113330/ 2025, SMIS code: 351358, financed from European funds via the POCIDIF 2021-2027 Program.

---

### REFERENCES

- [1] M.K. Debe, Electrocatalyst approaches and challenges for automotive fuel cells. *Nature*, 486, 43-51 (2012).
- [2] M. Shao, *et al.* (2016). Electrocatalysts for oxygen reduction reaction. *Chemical Reviews*, 116, 3594-3657.
- [3] H.A. Gasteiger, *et al.* (2005). Activity benchmarks in polymer electrolyte fuel cells. *Applied Catalysis B*, 56, 9-35.

## Ultrasound-assisted biodiesel production from brown grease using WS<sub>2</sub> nanocatalyst

Z. A. Dargie<sup>1</sup>, O. Semenova<sup>1\*</sup>, L. Yadgarov<sup>1</sup>, F. Nakonechny<sup>1</sup>, S. Lugovskoy<sup>1</sup>

1) Ariel University, Israel

\* olgasem AT ariel.ac.il

### Abstract

Biodiesel is a promising renewable alternative to fossil fuels; however, the high cost of edible oil feedstocks limits its large-scale implementation[1]. Brown grease (BG), a waste-derived lipid resource, is a low-cost, sustainable alternative, though its high free fatty acid content poses significant processing challenges[2]. This study investigates nanostructured tungsten disulfide (WS<sub>2</sub>) as a heterogeneous catalyst for ultrasound-assisted biodiesel production from BG. WS<sub>2</sub> exhibits high thermal and chemical stability, resistance to deactivation, and a layered structure with abundant catalytically active edge sites, enabling enhanced adsorption and accelerated reaction kinetics[3].

The catalyst was characterized and evaluated in simultaneous esterification and transesterification reactions, and key process parameters including temperature, reaction time, catalyst loading, and methanol to oil molar ratio were systematically optimized. Under ultrasonic irradiation at 80 kHz and 100 W, the biodiesel yield increased with temperature, reaching about 74% at 80 °C within 1 hr. Increasing the methanol content further improved conversion, with optimal performance observed at an oleic acid to methanol ratio of 1:141. Catalyst loading studies identified 16 wt. % WS<sub>2</sub> as optimal. Notably, particle size reduction through ball milling significantly enhanced catalytic performance, and under optimized conditions the milled catalyst achieved a maximum biodiesel yield of about 92%.

The enhanced catalytic activity is attributed to the high surface area and tunable electronic properties of nanoscale WS<sub>2</sub>, combined with cavitation-induced micro-mixing effects generated during sonication[4]. The proposed approach offers a scalable and economically attractive pathway for waste-to-energy conversion[5]. These findings highlight the strong potential of WS<sub>2</sub>-based nanocatalysts for advancing sustainable biodiesel production technologies.

---

**KEYWORDS:** Biodiesel, Brown grease, WS<sub>2</sub> nanocatalyst, Ultrasound-assisted reaction, Heterogeneous catalysis

---

**ACKNOWLEDGEMENTS:** This research was supported by Ariel University, which also provided funding for conference participation.

### REFERENCES

- [1] F. A. Plazas-Niño, N. R. Ortiz-Pimiento, and E. G. Montes-Páez, “National energy system optimization modelling for decarbonization pathways analysis: A systematic literature review,” *Renewable and Sustainable Energy Reviews*, vol. 162, p. 112406, Jul. 2022, doi: 10.1016/J.RSER.2022.112406.
- [2] M. Kolet, D. Zerbib, F. Nakonechny, and M. Nisnevitch, “Production of Biodiesel from Brown Grease,” 2020.
- [3] O. Semenova, Z. A. Dargie, L. Yadgarov, F. Nakonechny, and M. Nisnevitch, “Esterification of Free Fatty Acids Under Heterogeneous Catalysis Using Ultrasound,” *Catalysts*, vol. 15, no. 12, pp. 1-14, 2025, doi: 10.3390/catal15121161.
- [4] Y. D. Bizualem and A. G. Nurie, “A review on recent biodiesel intensification process through cavitation and microwave reactors: Yield, energy, and economic analysis,” *Heliyon*, vol. 10, no. 2, p. e24643, 2024, doi: 10.1016/j.heliyon.2024.e24643.
- [5] S. Ao, B. Changmai, C. Vanlalveni, M. V. L. Chhandama, A. E. H. Wheatley, and S. L. Rokhum, “Biomass waste-derived catalysts for biodiesel production: Recent advances and key challenges,” *Renew. Energy*, vol. 223, no. December 2023, p. 120031, 2024, doi: 10.1016/j.renene.2024.120031.

## Impact of the physicochemical properties of titanium dioxide nanoparticles on the absorption efficiency in rapeseed (*brassica napus* L.)

V. Kolbjonoks<sup>1</sup>\*, A. Petjukevičs<sup>1</sup>, M. Krasovska<sup>1</sup>, F. J. S. Valdez<sup>2</sup>, N. Škute<sup>1</sup>

1) *Daugavpils University, Latvia*

2) *Institute of Technology and Superior Studies of Monterrey, Mexico*

\* vadims.kolbjonoks AT du.lv

The rapid integration of nanotechnology into the agrochemical sector inevitably increases the risk of metallic nanomaterial accumulation in soil substrates. Titanium dioxide (TiO<sub>2</sub>) is one of the most prevalent anthropogenic agents in the environment. Understanding the absorption and transport mechanisms of these particles in plants is critical for assessing ecological risks and the safety of food chains. The aim of this study is to quantitatively and qualitatively evaluate the absorption of TiO<sub>2</sub> nanoparticles by the root system of rapeseed, as well as to analyze the patterns of their systemic translocation into the aerial organs of the plant.

The study was conducted under controlled soil conditions (pot experiment). Plants were exposed to TiO<sub>2</sub> nanoparticle suspensions (particle size 20-50 nm) at various concentrations: 0, 50, and 100 ml/L. The analysis assessed the impact of the nanomaterials on plant physiological parameters and their accumulation dynamics in various plant tissues. The results demonstrate the capacity of *Brassica napus* L. to absorb TiO<sub>2</sub> nanoparticles from the soil environment. It was found that absorption efficiency is directly dependent on the degree of nanoparticle dispersion and their concentration in the substrate. Despite morphological barriers in the plants, a portion of the nanoparticles successfully migrates through the xylem vessels, reaching vegetative organs.

---

**KEYWORDS:** Rapeseed, *Brassica napus* L, Titanium dioxide, Absorption, Translocation

## Numerical study of the effect of boron on oxygen vacancy stability and migration in ZnO electron-transport layers for perovskite solar cells

E. Len<sup>1, 2 \*</sup>, O. Kazakova<sup>3</sup>, M. Varvarin<sup>2</sup>, I. Galstian<sup>1</sup>

1) G. V. Kurdyumov Institute for Metal Physics, N.A.S. of Ukraine, 36 Academician Vernadsky Blvd., UA-03142 Kyiv, Ukraine

2) Kyiv Academic University, N.A.S. and M.E.S. of Ukraine, 36 Acad. Vernadsky Blvd., UA-03142 Kyiv, Ukraine

3) Chuiko Institute of Surface Chemistry, NAS of Ukraine, Ukraine

\* len.evgeniy AT gmail.com

The long-term stability of the ZnO/perovskite interface remains a major challenge for the commercialization of corresponding perovskite solar cells. Oxygen vacancies ( $V_O$ ) at the ZnO are considered to play an important role in interfacial degradation by introducing trap states and affecting defect-assisted ion migration.

The aim of this study is to theoretically evaluate the effectiveness of interstitial boron ( $B_i$ ) as a passivating agent for neutral and charged ( $2+$ ) oxygen vacancies in ZnO. We focus on understanding the formation energetics and stability of defect complexes and the kinetic impact of  $B_i$  on vacancy migration. All calculations were performed within the DFT framework using the Quantum ESPRESSO package [1]. The exchange-correlation potential was treated using PBE +  $U$  (with  $U = 7.5$  eV on Zn). The CI-NEB method [2] was employed to determine the minimum energy paths and activation barriers for vacancy diffusion.

Our calculations show that boron atoms energetically prefer to occupy sites adjacent to oxygen vacancies, forming stable complexes with a binding energy of -1.6 eV. PDOS analysis indicates that boron doping effectively shifts the vacancy-induced deep levels toward the conduction band edge. Furthermore, CI-NEB results suggest that boron not only electronically passivates defects but also physically "anchors" them in the lattice. Thus, interstitial boron acts as a dual-action stabilizer for ZnO. Interstitial boron provides energetic passivation through defect complex formation and kinetic stabilization by suppressing vacancy migration, making it a promising defect-engineering element for high-stability perovskite-based optoelectronics.

---

**KEYWORDS:** ZnO electron-transport layer, Oxygen vacancy migration, Boron doping, Perovskite solar cells, DFT calculations

---

**ACKNOWLEDGEMENTS:** This work was supported by the project No. 0123U102275 of the National Academy of Sciences of Ukraine.

---

### REFERENCES

- [1] P. Giannozzi, O. Andreussi, T. Brumme, O. Bunau, M. Buongiorno Nardelli, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, M. Cococcioni, N. Colonna, I. Carnimeo, A. Dal Corso, S. de Gironcoli, P. Delugas, R.A. DiStasio Jr., A. Ferretti, A. Floris, G. Fratesi, G. Fugallo, R. Gebauer, U. Gerstmann, F. Giustino, T. Gorni, J. Jia, M. Kawamura, H.-Y. Ko, A. Kokalj, E. Küçükbenli, M. Lazzeri, M. Marsili, N. Marzari, F. Mauri, N.L. Nguyen, H.-V. Nguyen, A. Otero-de-la-Roza, L. Paulatto, S. Poncè, D. Rocca, R. Sabatini, B. Santra, M. Schlipf, A.P. Seitsonen, A. Smogunov, I. Timrov, T. Thonhauser, P. Umari, N. Vast, X. Wu, and S. Baroni, "Advanced capabilities for materials modelling with Quantum ESPRESSO", *J. Phys.: Condens. Matter*, 29, 465901 (2017).
- [2] G. Henkelman, B.P. Uberuaga, and H. Jónsson, "A climbing image nudged elastic band method for finding saddle points and minimum energy paths", *J. Chem. Phys.*, 113, 9901-9904 (2000).

## Fe<sub>3</sub>O<sub>4</sub> nanoparticles treatment of wheat can reduce the oxidative stress caused by flooding and increased vitality

N. Škute<sup>1</sup>\*, A. Petjukevičs<sup>1</sup>, A. Čerkesa<sup>1</sup>, A. Batjuka<sup>1</sup>, V. Kolbjonoks<sup>1</sup>

1) Daugavpils University, Latvia

\* natalja.skute AT du.lv

The climatic variability result in plants being exposed to multiple abiotic stresses. Flooding is one of the major abiotic stresses affecting crop productivity. Nanoparticles can accumulate in plant roots and tissues and disrupting nutrient uptake, reducing growth. However, some nanoparticles can enhance plant resistance to abiotic stress. Wheat is one of the most important crops in the world. Therefore, the goal of this work was to study effect of Fe<sub>3</sub>O<sub>4</sub> nanoparticles on flooding stress resistance in the wheat (*Triticum aestivum* L.), using as stress markers as a fermentative and nonfermentive antioxidants, and the functioning of photosystem and photosynthetic pigments as a plant vitality indicator.

Four groups of plants were formed: control plants without nanoparticle treatment and flooding, control plants without nanoparticle treatment, but with flooding, plants with nanoparticle treatment with flooding and plants with nanoparticle treatment but without flooding. The plants were cultivated in a Environmental Climate Chamber (Sanyo, Japan) under controlled conditions. Fe<sub>3</sub>O<sub>4</sub> NPs were applied daily by watering the plants with aqueous NP suspensions at concentrations of 50 mg/L. To induce flooding stress, the pots were placed in trays filled with water to a level of 2 cm above the substrate surface. The Fe<sub>3</sub>O<sub>4</sub> nanoparticles were synthesized using the Massart method. Superoxide dismutase (SOD) was analyzed by spectrophotometry. The concentrations of chlorophyll (Chl a, Chl b) and total carotenoids were determined spectrophotometrically UV-Vis pulse spectrophotometer (DeNovix DS-7, US). Photochemical activity of photosystem II (PSII), as determined through chlorophyll a fluorescence analysis. Chlorophyll fluorescence was measured using Chlorophyll Fluorometer, OS-30p, OPTI-SCIENCES, US. Proteins accumulation was determined by fluorometry (Invitrogen Qubit fluorimeter). It was shown, that in control plants without nanoparticle treatment under flooding, SOD activity increased by 22% compared to the control without flooding but the treatment of plants with nanoparticles reduced the stress caused by flooding by a factor of two, also the carotenoid content in wheat under flooding in the control plants increased by 23% compared to the control without flooding, while in the nanoparticle treatment plants, under flooding the carotenoid content increased only by 15%. The chlorophyll a/b ratio and Fv/Fm was increased in the nanoparticle treatment plant group under flooding conditions, which indicates that nanoparticle treatment under these conditions can contribute stabilization of photosynthetic pigments. Protein accumulation in wheat root of nanoparticle treatment plant group under flooding conditions was increased by 50%.

Fe<sub>3</sub>O<sub>4</sub> Nanoparticles treatment of wheat can reduce the oxidative stress caused by flooding and increased protein accumulation and vitality. The results of this study confirm the potential of Fe<sub>3</sub>O<sub>4</sub> nanoparticles for practical applications.

---

**KEYWORDS:** Crops, Fe 3, O 4, Chlorophyll, SOD

---

### REFERENCES

- [1] El-M.M. Saber, A.A. Mahdi, A.H. Hassan, K.Y. Farroh, & Osman, A.. Effects of magnetite nanoparticles on physiological processes to alleviate salinity induced oxidative damage in wheat. *Journal of the Science of Food and Agriculture*, 101(13), 5550-5562, 2021
- [2] Y. Feng, V.D. Kreslavski, A.N. Shmarev, A.A. Ivanov, S.K. Zharmukhamedov, A. Kosobryukhov, M. Yu, S.I. Allakhverdiev, S. Shabala, Effects of iron oxide nanoparticles (Fe<sub>3</sub>O<sub>4</sub>) on growth, photosynthesis, antioxidant activity and distribution of mineral elements in wheat (*Triticum aestivum*) plants. *Plants*, 11(14), 1894. 2022 (2022).

## Tuning the exceptional reactivity of CeO<sub>2</sub> nanomaterials for decontamination

M. Stastny<sup>1</sup>, P. Rysanek<sup>2</sup>, J. Cundrle<sup>1</sup>, M. Dubovsky<sup>1</sup>, Z. Nemeckova<sup>1</sup>, J. Henych<sup>1\*</sup>

1) Institute of Inorganic Chemistry, Czech Academy of Sciences, Czech Republic

2) J.E. Purkyně University in Ústí nad Labem, Czech Republic

\* henych AT iic.cas.cz

Nanocrystalline cerium dioxide (CeO<sub>2</sub>, nanoceria) stands out in environmental catalysis [1] due to its unique surface chemistry [2], valence fluctuations (Ce<sup>3+</sup>/Ce<sup>4+</sup>), and enzyme-mimicking activities. This work explores the fundamental relations between defect engineering in ceria and its exceptional performance in capturing and destroying highly resilient toxic molecules. By optimizing low-temperature synthesis routes [3], we successfully maximize the density of surface hydroxyl groups and oxygen vacancies, which drive spontaneous hydrolytic and nucleophilic pathways at ambient temperature without external UV illumination. To translate these outstanding powder properties into scalable applications and prevent nanoparticle agglomeration, the engineered CeO<sub>2</sub> was immobilized into polymeric nanofiber matrices via conventional electrospinning and high-throughput hybrid spinning. The fundamental reactivity of the oxide—specifically its phosphatase-like activity—was verified through the rapid nucleophilic cleavage of stable bonds in widely used agrochemicals, such as the insecticide chlorpyrifos and glyphosate formulations (Roundup). Beyond pesticides, the extraordinary versatility of CeO<sub>2</sub> surface sites was proven by the successful degradation of critical emerging pollutants, including sulfonamide antibiotics [4] and sulfonylurea herbicides or chemical warfare agents [3]. Analytical tracking using operando DRIFTS [5] and HPLC/DAD/MS [3,4] demonstrates that the materials achieve simultaneous high-capacity adsorption and immediate chemical neutralization into non-toxic fragments. This study highlights how tailoring the intrinsic defect chemistry of CeO<sub>2</sub>-based materials and their integration into fibrous mats offers an interesting solution for advanced water purification.

**KEYWORDS:** Nanoceria, Nanofibrous membrane, Pesticides, Surface chemistry, Environmental catalysis

**ACKNOWLEDGEMENTS:** The project SQ01020060 (Sustainable filtration systems eliminating pesticides and other hazardous substances), which is co-financed with the state support of the Technology Agency of the Czech Republic within the Environment for Life 2 Programme, is gratefully acknowledged.

### REFERENCES

- [1] T. Montini, M. Melchionna, J. Kaspar and P. Fornasiero, “Fundamentals and Catalytic Applications of CeO<sub>2</sub>-Based Materials”, *Chem. Rev.*, 116, 5987 (2016).
- [2] J. Paier, C. Penschke and J. Sauer, “Oxygen Defects and Surface Chemistry of Ceria”, *Chem. Rev.*, 113, 3949 (2013).
- [3] J. Henych, M. Šťastný, J. Ederer, Z. Němečková, A. Pogorzelska, J. Tolasz, M. Kormunda, P. Ryšánek, B. Bazanów, D. Stygar, K. Mazanec and P. Janoš, “How the surface chemical properties of nanoceria are related to its enzyme-like, antiviral and degradation activity”, *Envi. Sci.: Nano*, 9, 3485 (2022).
- [4] J. Henych, M. Šťastný, S. Kříženecká, J. Čundrle, J. Tolasz, T. Dušková, M. Kormunda, J. Ederer, P. Ryšánek, V. Neubertová and P. Janoš, “Ceria-Catalyzed Hydrolytic Cleavage of Sulfonamides”, *Inorg. Chem.*, 63, 2298 (2024).
- [5] T. Dušková, Z. Němečková, J. Ederer, P. Ryšánek, M. Šťastný, and J. Henych, “Operando DRIFTS and NMR Spectroscopy Study of Hydrolytic and Photoinduced Transformations of Dimethyl Succinate on TiO<sub>2</sub> and CeO<sub>2</sub>”, *ACS EST Engg.*, 6, 1382 (2026).

## Engineering CeO<sub>2</sub>-based hybrid nanomaterials for dark and solar-driven degradation of emerging water pollutants

M. Stastny<sup>1\*</sup>, K. Kirakci<sup>1</sup>, M. Dubovsky<sup>1</sup>, J. Cundrle<sup>1</sup>, P. Rysanek<sup>2</sup>, J. Henych<sup>1</sup>

1) Institute of Inorganic Chemistry, Czech Academy of Sciences, Czech Republic

2) J.E. Purkyně University in Ústí nad Labem, Czech Republic

\* stastny AT iic.cas.cz

The increasing occurrence of persistent organic pollutants in aquatic environments, including endocrine disruptors, pharmaceuticals, pesticides and herbicides, necessitates the development of advanced materials for sustainable water remediation [1].

Among various semiconductor systems, nanocrystalline CeO<sub>2</sub> has attracted considerable attention owing to its unique redox flexibility, oxygen-vacancy-rich structure, and ability to operate under both illuminated and dark conditions.

Our research focuses on the development of CeO<sub>2</sub>-based hybrid nanomaterials designed to integrate photocatalytic activity with intrinsic dark-phase reactivity. Particular attention is devoted to photocatalytically active systems incorporating graphene oxide, g-C<sub>3</sub>N<sub>4</sub>, Ce-Bi mixed oxides/oxynitrates, metal diborides (MB<sub>2</sub>), molybdenum cluster-modified nanoceria and membrane-supported CeO<sub>2</sub> architectures. The engineered heterointerfaces promote efficient charge separation, extend light absorption, suppress electron-hole recombination, and enhance the generation of reactive oxygen species, resulting in improved degradation of organic contaminants under UV and solar irradiation.

Beyond their photocatalytic performance, CeO<sub>2</sub>-based materials exhibit a unique capability for pollutant transformation in the absence of illumination. Oxygen vacancies, reversible Ce<sup>3+</sup>/Ce<sup>4+</sup> redox cycling, and highly reactive surface sites enable reactive adsorption and catalytic hydrolysis processes that initiate contaminant degradation even under dark conditions. This dual-mode behavior distinguishes ceria-based systems from conventional photocatalysts and broadens their applicability under realistic environmental conditions.

The developed materials were successfully applied to the degradation of bisphenol analogues (BPA, BPS, and BPF), organophosphate esters, sulfonamide antibiotics, and other environmentally relevant contaminants. The results demonstrate that rational engineering of CeO<sub>2</sub>-based hybrid interfaces enables synergistic integration of dark-phase catalytic activity and solar-driven photocatalysis within a single multifunctional remediation platform [2-5]. Collectively, these studies demonstrate that rational engineering of CeO<sub>2</sub>-based hybrid interfaces enables seamless integration of dark- and light-driven degradation pathways within a single multifunctional remediation platform.

**KEYWORDS:** Ceria-based hybrids, Dark-phase catalysis, Solar photocatalysis, Reactive oxygen species, Emerging pollutants

**ACKNOWLEDGEMENTS:** This work was funded by Czech Science Foundation through project 25-15972S, which is hereby acknowledged. The work was also supported by the Czech Academy of Sciences Strategy AV21 scheme as part of "The power of objects: Materiality between past and future" grant at the Institute of Inorganic Chemistry of the Czech Academy of Sciences.

### REFERENCES

- [1] A.O. Adeola, B.A. Abiodun, D.O. Adenuga, and P.N. Nomngongo, "Adsorptive and photocatalytic remediation of hazardous organic chemical pollutants in aqueous medium: A review", *J. Contam. Hydrol.* 248, 104019 (2022).
- [2] J. Henych, P. Ryšánek, M. Štátný, Z. Němečková, S. Adamec, M. Kormunda, S. Kamínková, K. Hamalová, J. Tolasz, and P. Janoš, "Electrospun PA6 Nanofibers Bearing the CeO<sub>2</sub> Dephosphorylation Catalyst", *ACS Omega.* 8, 26610-26618 (2023).
- [3] J. Henych, M. Štátný, S. Kříženecká, J. Čundrle, J. Tolasz, T. Dušková, M. Kormunda, J. Ederer, Š. Stehlík, P. Ryšánek, V. Neubertová, and P. Janoš, "Cerium-Catalyzed Hydrolytic Cleavage of Sulfonamides", *Inorg. Chem.* 63, 2298-2309 (2024).
- [4] M. Štátný, D. Bovol, J. Tolasz, P. Bezdička, J. Čundrle, M. Kormunda, I. Dimitrov, P. Janoš, K. Kirakci, and J. Henych, "Interfacial behavior of ceria grown on graphene oxide and its use for hydrolytic and photocatalytic decomposition of bisphenols A, S, and F", *Environ. Sci. Nano.* 12, 502-513 (2025).
- [5] M. Štátný, J. Tolasz, D. Bovol, M. Kloda, Y. Sugahara, K. Lang, J. Henych, and K. Kirakci, "Concerted Reactive Adsorption and Photocatalytic Degradation of Bisphenol-S on Molybdenum Cluster-Modified Nanoceria", *Inorg. Chem.* 64, 18166-18174 (2025).

## Nanoceria as molecular scissors: Hydrolytic cleavage of environmentally and biologically relevant compounds

J. Čundrle<sup>1</sup>\*, M. Stastny<sup>2</sup>, J. Henych<sup>2</sup>

1) Faculty of Environment, Jan Evangelista Purkyně University in Ústí nad Labem, Pasteurova 3632/15, 400 96 Ústí nad Labem, Czech Republic, Czech Republic

2) Institute of Inorganic Chemistry, Czech Academy of Sciences, Czech Republic

\* honzacundrle AT seznam.cz

Nanoceria (CeO<sub>2</sub>) has attracted considerable interest owing to its unique redox and acid-base properties, high oxygen mobility, tunable surface chemistry and cost-effectiveness. These features make it a versatile material for applications in catalysis, environmental remediation, and nanozyme technologies. In recent years, increasing attention has been paid to its ability to promote hydrolytic bond cleavage under mild conditions. While most studies have focused on the degradation of organophosphorus compounds, including pesticides [1] and chemical warfare agents [2], recent work has shown that amide-containing substrates, such as sulfonamide antibiotics [3], are also highly susceptible to CeO<sub>2</sub>-catalyzed hydrolysis, highlighting the potential of nanoceria for selective amide bond cleavage.

In this contribution, nanocrystalline CeO<sub>2</sub> materials prepared by precipitation methods were synthesized and comprehensively characterized using a range of structural and surface-sensitive techniques, with special focus on their acid-base properties and their role in catalytic hydrolysis. We demonstrate that nanoceria is capable of promoting the hydrolysis of various amide-containing compounds, including sulfonylurea herbicides, β-lactam antibiotics, and peptide-based substrates, under ambient conditions and in the absence of any external activation. Particular attention is devoted to establishing structure-activity relationships, elucidating reaction pathways, and understanding the factors governing bond-cleavage selectivity.

The obtained results provide new insights into the catalytic behaviour of CeO<sub>2</sub> towards environmentally relevant pollutants and biologically important molecules. Beyond applications in water treatment, the demonstrated ability of nanoceria to promote selective cleavage of amide bonds opens opportunities for the development of artificial nanozymes and advanced catalytic systems for pharmaceutical and biotechnological processes.

---

**KEYWORDS:** Nanoceria materials, Hydrolytic catalysis, Water pollutants, Peptide cleavage, Nanozymes

---

**ACKNOWLEDGEMENTS:** Projects no. UJEP-IGA-2026-53-005-2 (CeO<sub>2</sub>/Metal Carbides Hybrid Nanostructures for Advanced Functional Materials), funded by UJEP Internal Grant Agency, and no. UJEP-SGS-2025-44-002-3 (Study of hydrolytic decomposition reactions on the surface of CeO<sub>2</sub>), funded by UJEP Student's Grant Competition, are both gratefully acknowledged.

---

### REFERENCES

- [1] J. Tolasz, J. Henych, M. Šťastný, Z. Němečková, M. Š. M. Š. Slušná, T. Opletal, and P. Janoš, "Room-temperature synthesis of nanoceria for degradation of organophosphate pesticides and its regeneration and reuse", *RSC Advances*, 10, 14441-14450 (2020).
- [2] P. Janoš, J. Henych, O. Pelant, V. Pilařová, L. Vrtoch, M. Kormunda, K. Mazanec, and V. Štengl, "Cerium oxide for the destruction of chemical warfare agents: A comparison of synthetic routes", *Journal of Hazardous Materials*, 304, 259-268 (2016).
- [3] J. Henych, M. Šťastný, S. Kříženecká, J. Čundrle, J. Tolasz, T. Dušková, M. Kormunda, J. Ederer, Š. Stehlík, P. Ryšánek, V. Neubertová, and P. Janoš, "Ceria-Catalyzed Hydrolytic Cleavage of Sulfonamides", *Inorganic Chemistry*, 63(4), 2298-2309 (2024).

## High-energy processing modification of carbon-containing composites based on light metals for alternative energy

H. Mykhailova<sup>1\*</sup>, E. Len<sup>1,2</sup>, S. Mulenko<sup>1</sup>, M. Rud<sup>1</sup>, T. Vladimirova<sup>3</sup>, Y. Vasylyk<sup>3</sup>

1) G. V. Kurdyumov Institute for Metal Physics, N.A.S. of Ukraine, 36 Academician Vernadsky Blvd., UA-03142 Kyiv, Ukraine

2) Kyiv Academic University, N.A.S. and M.E.S. of Ukraine, 36 Acad. Vernadsky Blvd., UA-03142 Kyiv, Ukraine

3) G. V. Kurdyumov Institute for Metal Physics, N.A.S. of Ukraine, 36 Academician Vernadsky Blvd., UA-03142 Kyiv, Ukraine, Ukraine

\* mihajlova.halina AT gmail.com

Today, many areas of nanotechnology are associated with carbon nanomaterials and are focused on the development of advanced materials for various industrial applications, including energy storage and energy conversion systems. However, a number of challenges still hinder the widespread implementation of alternative energy technologies. These include high cost, operational complexity, and degradation of materials used in thermionic energy converters (TECs). Conventional TECs based on refractory metals provide high electron emission current density only at elevated temperatures typical of nuclear reactors or high-temperature combustion environments. Therefore, for broader practical application of direct energy conversion systems, it is necessary to significantly reduce the operating temperature of TEC cathodes while maintaining their electron emission performance to a level achievable using moderate heat sources such as household-scale heat generators or solar concentrators.

This work is devoted to the synthesis and optimization of titanium-based composites with different contents of carbon nanotubes (CNTs). CNTs with a diameter of  $18 \pm 6$  nm were used. The composites were prepared by mechanochemical synthesis, followed by compaction under pressures of 3-4 MPa.

To evaluate the suitability of these materials as cathodes for energy converters, information on the surface state and structure of the investigated materials is required. Laser processing enables controlled modification of surface morphology, defect structure, and electronic properties, which can enhance electrochemical activity, electrical conductivity, and operational stability. Therefore, the samples were subjected to laser annealing at 200 °C, 360 °C, and 400 °C with a holding time of 10 minutes in both vacuum and air atmospheres.

X-ray diffraction analysis revealed that the samples contain  $\alpha$ -Ti, titanium oxide, titanium carbide, and carbon phases. With increasing annealing temperature, a decrease in oxide and carbon-related phases was observed, which can be attributed to complex surface processes induced by thermal and laser treatment, including phase transformations and interfacial reactions. Microscopic studies showed significant surface modification after annealing, characterized by the formation of a complex, multicomponent, and non-uniform surface structure.

The obtained results demonstrate that titanium-based CNT composites are promising candidates for cathode materials in low-temperature thermionic energy converters.

---

**KEYWORDS:** Ti-carbon nanocomposites, Carbon nanotubes, Titanium powder, Electrophysical properties, Laser annealing

---

**ACKNOWLEDGEMENTS:** This work was supported by the project No. 0123U102275 of the National Academy of Sciences of Ukraine.

## Evaluating the degree of supercooling in erythritol-based Al<sub>2</sub>O<sub>3</sub> and TiO<sub>2</sub> nanofluids

Y. Hlek<sup>1,2\*</sup>, V. Zhelezny<sup>3</sup>, D. Ivchenko<sup>3</sup>, V. Khalak<sup>3</sup>, B. Kvasnytskyi<sup>3</sup>, O. Khliyeva<sup>4</sup>

1) Odessa National Maritime University, Ukraine

2) Odessa State Academy of Civil Engineering and Architecture, Odesa, Ukraine

3) Odessa National University of Technology, Ukraine

4) National University “Odessa Maritime Academy”, Ukraine

\* yanaglek90 AT gmail.com

The use of erythritol as a thermal energy storage material is limited by its susceptibility to pronounced supercooling. Thermograms were used to experimentally study the effect of nanoparticles on this phenomenon. Analysis of the obtained thermograms shows that the addition of Al<sub>2</sub>O<sub>3</sub> and TiO<sub>2</sub> nanoparticles, contrary to theoretical concepts regarding the role of nucleators, initially appeared to increase the supercooling of nanofluids compared to pure erythritol. The authors attribute these effects to the influence of nanoparticles on the thermophysical properties of erythritol and an increase in the rate of temperature change during cooling.

The report demonstrates that Al<sub>2</sub>O<sub>3</sub> and TiO<sub>2</sub> nanoparticles increase the density, thermal conductivity, and viscosity of erythritol while decreasing its specific heat. These altered thermophysical properties accelerate the cooling rate, leading to greater supercooling.

The authors concluded that a direct experimental study of the degree of supercooling and a simple comparison of supercooling values between the base material and nanofluids are insufficiently accurate, since the cooling process occurs at different rates. At higher cooling rates, nanofluids “pass” the point of equilibrium phase transition faster than stable crystallization centers can form. This effect leads to the false conclusion that nanoparticles are ineffective in reducing the supercooling of erythritol.

An analysis of the dependence of supercooling on the normalized cooling rate showed that this value is actually lower for erythritol-based nanofluids than for the pure substance. The method used for processing thermograms confirms that Al<sub>2</sub>O<sub>3</sub> and TiO<sub>2</sub> nanoparticles serve as centers of heterogeneous nucleation. At concentrations of 1.1 % and 1.13 %, the introduction of additives reduces the supercooling value by approximately 5-6 °C. The results demonstrate the effectiveness of using these nanoparticles to initiate crystallization when experimental data is correctly interpreted.

---

**KEYWORDS:** Thermal energy storage, Erythritol, Nanoparticles, Supercooling

# Track 11

Nanobiomedical Research and Translational Applications

## Engineering dynamic nanobiomaterial interfaces for controlled biointeractions and functional stability

S. Minko<sup>1\*</sup>

1) University of Georgia, USA

\* sminko AT uga.edu

Advances in nanobiomaterials have enabled unprecedented control over biological interactions at interfaces, offering new strategies for regulating cellular behavior and biomolecular function. This presentation provides an overview of our research on the design of dynamic and stimuli-responsive nanostructured systems [1] that modulate interactions between synthetic materials and biological entities. By integrating principles of polymer chemistry, interfacial engineering, and biomolecular stabilization, we develop functional materials capable of selectively controlling adhesion, activity, and stability in complex biological environments.

Key contributions include the development of nanostructured interfaces for label-free manipulation and sorting of particulates [3], as well as nonenzymatic strategies for cell harvesting through decoupling of adhesive and disjoining interactions [2]. In parallel, we explore molecular brush architectures for enhancing the thermal and operational stability of enzymes, enabling robust catalytic performance under otherwise denaturing conditions [4], [5]. These approaches highlight the role of nanoscale architecture and interfacial dynamics in dictating biological outcomes.

Collectively, this work establishes a versatile framework for engineering adaptive biointerfaces with tunable functionality. The insights gained provide new opportunities for applications in biocatalysis, regenerative medicine, and bioseparation technologies, bridging the gap between material design and biological performance.

---

**KEYWORDS:** Nanobiomaterials, Stimuli-Responsive interfaces, Biointerface engineering, Enzyme stabilization, Cell-Material interactions

---

**ACKNOWLEDGEMENTS:** The author acknowledges financial support from the US funding agencies: NSF (EAGER, CBET, and DMR grant programs), GRA and DOD. Support from ORNL and access to shared research facilities are also gratefully acknowledged. The author thanks collaborators and group members for their contributions to the development of nanobiomaterial platforms and biointerface engineering strategies presented in this work.

---

### REFERENCES

- [1] K. Peranidze, N.S. Yadavalli, B. Blevins, M. Parker, T. Jain, M. Aghajohari, S. Minko, V. Reukov, Strategies for fabricating aligned nano- and microfiber scaffolds: an overview for cell culture applications. *Nanoscale* 2025, 17 (36), 20670-20703.
- [2] Y. Kim, U.M. Jahan, A.P. Deltchev, N. Lavrik, V. Reukov, S. Minko, Strategy for nonenzymatic harvesting of cells via decoupling of adhesive and disjoining domains of nanostructured stimulus-responsive polymer films. *ACS Appl. Mater. Interfaces* 2023, 15 (42), 49012-49021.
- [3] Y. Kim, A.M. Laradji, S. Sharma, W. Zhang, N.S. Yadavalli, J. Xie, V. Popik, S. Minko, Refining of Particulates at Stimuli-Responsive Interfaces: Label-Free Sorting and Isolation. *Angew. Chem. Int. Ed.* 2022, 61, e202110990.
- [4] O. Kudina, A. Zakharchenko, O. Trotsenko, A. Tokarev, L. Ionov, G. Stoychev, N. Pureskiy, S.W. Pryor, A. Voronov, S. Minko, Highly efficient phase boundary biocatalysis with enzymogel nanoparticles. *Angew. Chem. Int. Ed.* 2014, 53 (2), 483-487.
- [5] A. Zakharchenko, N. Guz, A.M. Laradji, E. Katz, S. Minko, Magnetic Field Remotely Controlled Selective Biocatalysis. *Nature Catalysis* 2018, 1, 73-81.

## “Green” carbon dots and nanohybrids for theranostic application

V. Skryshevsky<sup>1\*</sup>, H. Kuznietsova<sup>1</sup>, N. Dziubenko<sup>1</sup>, O. Pylypova<sup>2</sup>, I. Lysenko<sup>1</sup>, K. Paliienko<sup>3</sup>, A. Topchylo<sup>3</sup>,  
I. Byelinska<sup>1</sup>, A. Zaderko<sup>4</sup>, V. Lysenko<sup>5</sup>

1) Taras Shevchenko National University of Kyiv, Ukraine

2) Institute of High Technologies, Taras Shevchenko National University of Kyiv, Ukraine

3) Corporation Science Park, Taras Shevchenko University of Kyiv, Ukraine

4) Université Lyon 1, CNRS, Institut Lumière Matière, France

5) Light Matter Institute, Claude Bernard University of Lyon/CNRS, France

\* skryshevsky AT knu.ua

Carbon dots (CDs) and their doped nanohybrids are zero-dimensional fluorescent nanoparticles that combine excellent biocompatibility, tunable photoluminescence, and ease of surface functionalization, making them highly attractive for nanobiomedicine. Green synthesis routes using renewable biowastes (coffee grounds, citric acid/urea) and simple solvothermal/microwave-assisted methods further enhance their sustainability while preserving low cost and minimal environmental impact. Recent advances have demonstrated that incorporation of paramagnetic Gd<sup>3+</sup> ions into fluorinated or coffee-waste-derived CDs yields multifunctional nanohybrids capable of simultaneous fluorescence imaging and magnetic resonance imaging (MRI) contrast enhancement, while retaining intrinsic photoacoustic, photothermal, and antimicrobial properties.

The key challenge for clinical translation of theranostic nanomaterials remains achieving high biocompatibility and multimodal functionality without toxicity after prolonged exposure. Here we show that “green” Gd<sup>3+</sup>-doped carbon dots and nanohybrids synthesized from biocompatible precursors exhibit ultrasmall sizes (2-10 nm or 40-80 nm aggregates), strong T<sub>1</sub>/T<sub>2</sub> MRI contrast across field strengths, bright multi-color fluorescence, and efficient cellular uptake into nuclei without altering cell viability in 3T3-L<sub>1</sub> and A<sub>549</sub> lines up to 1 mg/mL. In vivo studies in mice confirmed no significant lethality, normalized hematological and biochemical parameters, and minimal organ histopathology after repeated dosing. When combined with laser irradiation, these nanoparticles significantly slowed Lewis lung carcinoma growth and increased survival by >30 %, while topical application accelerated healing of phosphorus oxide-induced cutaneous burns via antimicrobial, anti-inflammatory, and cytoprotective effects [1].

These findings demonstrate that green-synthesized Gd-doped CDs overcome the toxicity limitations of conventional contrast agents and expand theranostic capabilities beyond imaging to include photoacoustic therapy and wound management. The results advance the development of safe, eco-friendly multimodal nanoproboscopes and open new avenues for personalized nanomedicine in oncology and regenerative therapies [2].

---

**KEYWORDS:** Carbon dots, Therapies, Antimicrobial effects, Hematological and biochemical parameters

---

**ACKNOWLEDGEMENTS:** This work was financially supported by EU Horizon 2020 Research and Innovation Staff Exchange Programme (RISE) under Marie Skłodowska-Curie Action (project “UNAT” No.101008159) and National Research Foundation of Ukraine (project 2025.07/0098).

---

### REFERENCES

- [1] P. Lishchuk, H. Kuznietsova, T. Dovbynychuk, N. Dziubenko, L. Garmanchuk, S. Alekseev, M. Isaiev, N. Pozdnyakova, A. Pastukhov, N. Krisanova, T. Borisova, V. Lysenko, V. Skryshevsky, Impact of irradiation conditions on therapy of Lewis lung carcinoma in mice using glucose-ethylenediamine carbon dots, *BMC Cancer*, 25, 39 (2025).
- [2] V. Lysenko, H. Kuznietsova, N. Dziubenko, I. Byelinska, A. Zaderko, T. Lysenko, and V. Skryshevsky, “Application of carbon dots as antibacterial agents: a mini review,” *BioNanoScience*, 14, 1819-1831 (2024).

## Cisplatin-crosslinked DNA nanoparticles for radiotherapeutic applications

L. Sala<sup>1</sup>\*, T. Perecko<sup>2</sup>, J. Pankrác<sup>3</sup>, J. Kočíšek<sup>1</sup>

1) J. Heyrovský Institute of Physical Chemistry of the CAS, Czech Republic

2) Institute of Biophysics of the CAS, Czech Republic

3) Center for Advanced Preclinical Imaging (CAPI), First Faculty of Medicine, Charles University, Czech Republic

\* leo.sala AT jh-inst.cas.cz

DNA nanostructures are promising carriers for multimodal theranostics due to their precise self-assembly and unparalleled functionalization site addressability; however, poor physiological stability remains a significant barrier to clinical translation [1]. In this work, we enhanced the stability of two DNA-based nanostructures: DNA nanoblocks (6x6x64 nt) [2] and condensed ssDNA scaffolds [3]. Both systems were stabilized using cisplatin, which serves as a dual-purpose cross-linking agent and chemotherapeutic/radiosensitizing payload [4]. Structural integrity was verified via Atomic Force Microscopy (AFM) and Transmission Electron Microscopy (TEM), while Inductively Coupled Plasma Mass Spectrometry (ICP-MS) quantified cisplatin loading. Cytotoxic evaluation revealed distinct performance profiles between the two platforms. Cisplatin-cross-linked DNA nanoblocks (CxDN) exhibited pronounced cytotoxicity at nanomolar concentrations in FaDu and MCF<sub>7</sub> cancer cell lines (MTT assay), supported by ICP-MS and fluorescence microscopy showing sustained intracellular platinum retention for up to 96 h. In contrast, fully cross-linked ssDNA scaffolds (CxSS) did not induce significant cytotoxicity in FaDu cells within 24 h. Furthermore,  $\gamma$ -irradiation survival assays demonstrated that both CxSS and CxDN effectively radiosensitized FaDu cells at high doses, whereas MCF<sub>7</sub> cells showed limited sensitization for CxDNs despite similar uptake, suggesting cell-line-specific modulation of radiation response.

In vivo biodistribution of IRDye<sub>800</sub>-labeled CxDN in nude mice showed rapid systemic clearance ( $t_{1/2} \approx 30$  min) with predominant accumulation in the liver and kidneys. Persistent ex vivo fluorescence up to 48 h suggests significant tissue retention before hepatobiliary and renal clearance. Overall, while cisplatin cross-linking successfully yields stable, multifunctional nanostructures with potent chemo-radiosensitizing activity, further surface modification is required to extend systemic circulation and improve targeting efficiency for clinical applications.

---

**KEYWORDS:** Nanobiomedicine, DNA nanotechnology, Radiotherapy

---

**ACKNOWLEDGEMENTS:** We acknowledge the support from the Czech Science Foundation grant no. 24-11503S, Ministry of Education, Youth, and Sports of the Czech Republic via project CZ.02.01.01/00/22\_008/0004649 QUEENTECH co-funded by the European Union, and the European Union’s Horizon Europe research and innovation programme under grant agreement number 101058620 canSERV.

---

### REFERENCES

- [1] A. Keller, and V. Linko, “Challenges and perspectives of DNA nanostructures in biomedicine”, *Angew. Chem. Int. Ed.*, 59,15818 (2020).
- [2] Y. F. Zhong, J. Cheng, Y. Liu, T. Luo, Y. Wang, K. Jiang, F. Mo, J. Song, “DNA nanostructures as Pt (IV) prodrug delivery systems to combat chemoresistance”, *Small*, 16, 2003646 (2020).
- [3] L. Sala, T. Perecko, A. Kaňa, J. Kočíšek, “Scalable synthesis of platinated DNA nanoparticles with radiosensitizing potential”, [preprint] Zenodo, <http://doi.org/10.5281/zenodo.19813732> (2026).
- [4] L. Sala, T. Perecko, O. Mestek, D. Pinkas, T. Homola, J. Kočíšek, “Cisplatin-Cross-Linked DNA Origami Nanostructures for Drug Delivery Applications”, *ACS Appl. Nano Mater.*, 5, 13267-13275 (2022).

## Harmonic response and heat dissipation effects of magnetic nanoparticles for theranostic applications

T. Sakamoto<sup>1</sup>, Y. Kusumoto<sup>1</sup>, N. Kataoka<sup>1</sup>, Y. Ichianagi<sup>1</sup>\*

*1) Department of Physics, Graduate School of Engineering Science, Yokohama National University, Yokohama, Kanagawa 240-8501, Japan, Japan*

\* yuko AT ynu.ac.jp

The true value of research on magnetic nanoparticles lies not only in fundamental physics but is also in its becoming increasingly evident application to fields with high societal demand, such as diagnostics, medicine, and the environment. Their use as contrast agents in magnetic resonance imaging (MRI) is a prime example of this, with research centered on iron oxide nanoparticles has advancing across the boundaries of materials science, physics, chemistry, and medicine.

In recent years, the biomedical field has been exploring “theranostics,” combining diagnosis and therapy [1, 2]. We have found that the nanoparticles we developed function as both diagnostic imaging tracers and as a hyperthermia therapy agents.

In this study, Gd and Zn doped Mn-ferrite NPs with various particle sizes and compositions were prepared using a wet-chemical method. Their local structures were analyzed by X-ray diffraction (XRD) and synchrotron X-ray absorption fine structure (XAFS) measurements. DC magnetization and AC magnetic susceptibility measurements were also performed.

Regarding its diagnostic properties,  $T_1$  and  $T_2$  relaxation measurements revealed that Gd-doped Mn-ferrite functions as an MRI contrast agent, demonstrating its diagnostic properties. To verify its effectiveness as a tracer for MPI, we measured the third-harmonic signal in an alternating magnetic field. Response intensity varied with particle size  $d$ . Particles with  $d = 10$  and  $14$  nm exhibited large responses, which decreased successively for particles for  $17$  and  $21$  nm. Particles exhibiting superparamagnetic behavior in the magnetization measurements showed large responses.

Samples of Gd-doped Mn-Zn ferrite with high magnetization and magnetic anisotropy exhibited high signal intensity at low frequencies. However, as the drive field frequency increased, the effect of magnetic anisotropy had a greater effect, and it was confirmed that Gd-doped Mn-Zn ferrite with a particle size of  $10.5$  nm had a signal intensity approximately 22 times that of the control at a drive field frequency of  $48$  kHz. For Gd doped Mn-ferrite particles  $14$  nm or larger, which had a high, heat generation exceeding  $42.5^\circ\text{C}$  ( $315.5$  K) -the temperature at which cancer cells die-was confirmed. The heat dissipation rate suggested that samples followed magnetic relaxation loss. This outcome supports their potential as a theranostic material enabling simultaneous treatment and diagnosis.

---

**KEYWORDS:** Magnetic nanoparticles, Theranostics, Imaging, Hyperthermia, XAFS

---

**ACKNOWLEDGEMENTS:** This study was partially supported by a grant for JST-Mirai JPMJMI17D7 from the Japan Science and Technology Agency, Japan Agency for Medical Research Development (AMED) No.H-48, and a Grand-in Aid for Science Research (No. 23656013, 25K01619) from the Japan Society for the Promotion of Science (JSPS).

---

### REFERENCES

- [1] D. Shigeoka, T. Yamazaki, T. Ishikawa, K. Miike, K. Fujiwara, T. Ide, A. Oshima, T. Hashimoto, D. Aihara, A. Usui, Y. Hosokai, H. Saito and Y. Ichianagi, “Functionalization and magnetics relaxation of ferrite nanoparticles for theranostics”, IEEE Transactions on Magnetism Vol.54,11 6100707 (2018)
- [2] H. Katayanagi, N. Sakai, S. Hamada, A. Usui, K. Aoki, K. Kodama, K. Nashimoto, Y. Hosokai, and Y. Ichianagi, “Magnetic relaxation and modification of thiol groups on Co-Mg ferrite nanoparticles for theranostics”, Chem. Nano. Mat. 202200014, 1-7 (2022)
- [3] N. Kataoka, A. Usui, Y. Kusumoto, H. Amano, and Y. Ichianagi, “Magnetic Relaxation of Gd-Doped MnFe<sub>2</sub>O<sub>4</sub> Nanoparticles for MR Effect and Heat Dissipation”, IEEE Trans. Magn., 61, 5400505 (2025)
- [4] T. Sakamoto, K. Nii, Y. Fujita, T. Moriwaki, H. Amano, R. Abe, and Y. Ichianagi, “Harmonic response of Gd-doped Mn-ferrite nanoparticles under AC magnetic field and optimization of Gd doping for MPI applications”, AIP Advances 14, 015241 (2024)

## Supracolloidal assemblies of gold nanoantennae for biosensing applications

L. Baraban<sup>1</sup> \*

1) Institute of Radiopharmaceutical Cancer Research, Helmholtz-Zentrum Dresden-Rossendorf e.V. (HZDR), 01328 Dresden, Germany

\* l.baraban AT hzdr.de

To date, plasmonic nanobiosensors mainly demonstrate relatively small resonance shifts accompanied with insufficient spectral resolution and peak discrimination, when detecting biomolecules. Addressing these challenges necessitates the development of new strategies and nanoarchitectures to enhance plasmonic performance. In this regard, exploring the self-assembly of varied geometric patterns, nanoparticle clusters, and ordered arrays of plasmonic metal nanostructures or nanoparticles has emerged as a promising solution. These architectures can give rise to additional resonant modes that are highly tunable and exhibit enhanced field confinement, resulting in stronger and narrower resonance signatures than those of single nanoparticles.

In this particular work we report the large area linear periodic assemblies of gold nanoparticles and evaluate their polarization-dependent biosensing performance through proof-of-concept studies. Two complementary fabrication strategies are investigated: (i) laser interference lithography (LIL), which enables high-fidelity patterning over moderate areas, and (ii) wrinkle-assisted patterning, a scalable and cost-effective alternative. Despite differences in structural morphology, both approaches deliver comparable sensing performance, highlighting the versatility and broad applicability of the proposed biosensing platform [1].

Sensor performance is first assessed using glycerol-water mixtures with well-defined refractive indices. Subsequently, the platform is biofunctionalized for the detection of antibodies against Tumor Necrosis Factor-Alpha, a pro-inflammatory cytokine closely associated with cancer progression and prognosis. Plasmonic resonance peak shifts of the AuNP assemblies are monitored throughout the functionalization and detection processes using polarized visible-near-infrared (vis-NIR) spectroscopy.

The results reveal a pronounced polarization-dependent plasmonic response, characterized by significant resonance wavelength shifts ( $\Delta\lambda$ ). In particular, the longitudinal plasmon mode exhibits up to a fivefold signal enhancement compared with the transverse mode, a trend consistently observed for both LIL- and wrinkle-based templates. These findings demonstrate a promising supracolloidal nanostructuring strategy for the scalable fabrication of highly sensitive plasmonic biosensors and biochip platforms.

---

**KEYWORDS:** Gold nanoparticles, Plasmonic biosensors, Supracolloidal assemblies

---

**ACKNOWLEDGEMENTS:** Larysa Baraban acknowledges the financial support of German Research Foundation for the funding of GRK 2767 - 'Supracolloidal Structures' and grant number BA 4986/10. Furthermore, she acknowledges the financial support of the project ImmunoChip, which has received funding from the European Research Council (ERC) under the European Union's Horizon Europe research and innovation program grant agreement No 101045415.

---

### REFERENCES

- [1] T.H. Tonmoy, S. Seçkin, M. Hoffmann, *et al.*, Enhanced Refractive Index Sensitivity of Linearly Assembled Gold Nanoantennae for Biosensing Applications. *Small* 2026, 22 (9), e10159.

## Antibacterial application of ZnO, CuO and Y<sub>2</sub>O<sub>3</sub> nanomaterials

N. M. Mlinarić<sup>1\*</sup>, K. Živković<sup>2</sup>, A. Selmani<sup>3</sup>, A. Učakar<sup>4</sup>, E. Roblegg<sup>3</sup>, A. Stanković<sup>5</sup>

1) Ruđer Bošković Institute, Zagreb, Croatia

2) Faculty of Science, University of Zagreb, Zagreb, Croatia

3) University of Graz, Institute of Pharmaceutical Sciences, Pharmaceutical Technology & Biopharmacy, Graz, Austria

4) Jožef Stefan Institute, Jamova 39, SI-1001 Ljubljana, Slovenia, Slovenia

5) Josip Juraj Strossmayer University of Osijek, Osijek, Croatia

\* nmatijak AT irb.hr

More than 35,000 deaths each year in the EU, Iceland, and Norway are attributed to antimicrobial-resistant bacterial infections, highlighting the urgent need for alternative antimicrobial strategies. Unlike antibiotic-releasing coatings, metal oxide nanoparticles (NPs) offer sustained antimicrobial activity without promoting bacterial resistance. Owing to their durability, physicochemical stability, and relatively low cytotoxicity toward human cells, metallic NPs have emerged as promising candidates for antibacterial applications. In particular, CuO and ZnO nanoparticles have attracted significant attention due to their intrinsic antimicrobial properties and biological relevance as essential trace elements [1, 2].

Here, we showed that CuO, ZnO, and Y<sub>2</sub>O<sub>3</sub> NPs and multimetal (Cu, Zn, and Y) NPs with different sizes and morphologies exhibit different surface properties and show promising antibacterial activity against *Staphylococcus aureus* and *Escherichia coli*. We prepared nanoparticles with various anionic salts of Zn, Cu, and Y, stabilised with tannic acid during synthesis. The NPs exhibited different morphologies and were characterized by different nanoparticle sizes and distributions. The developed NPS exhibited promising antibacterial action against Gram-positive *Staphylococcus aureus* and Gram-negative *Escherichia coli*.

Our findings reveal that nanoparticle size, morphology, and surface composition play a critical role in determining antibacterial performance. This study provides valuable insight into the rational design of nanoparticles aimed at enhancing antimicrobial effectiveness. The results establish a foundation for the development of next-generation biocompatible antimicrobial materials for biomedical applications.

---

**KEYWORDS:** CuO nanoparticles, ZnO nanoparticles, Y<sub>2</sub>O<sub>3</sub> nanoparticles, Antibacterial application

---

**ACKNOWLEDGEMENTS:** The authors acknowledge the financial support from the UIP project BIO-METONIC, financed by the Croatian Science Foundation.

---

### REFERENCES

- [1] N. Matijaković Mlinarić, *et al.* Biocompatible Polyelectrolyte Multilayers with Copper Oxide and Zinc Oxide Nanoparticles for Inhibiting Bacterial Growth. *ACS Appl. Nano Mater.* 7, 12550-12563 (2024).
- [2] N. Matijaković Mlinarić, *et al.* Poly(Allylamine Hydrochloride) and ZnO Nanohybrid Coating for the Development of Hydrophobic, Antibacterial, and Biocompatible Textiles. *Nanomaterials* 14, 570 (2024).

## Nanoparticle-enzyme sensor: A new technology for low-cost, rapid point-of-care diagnostics

B. Bisht<sup>1, 1\*</sup>, V. Bhalla<sup>1</sup>

1) CSIR-Institute of Microbial Technology Chandigarh India, India

\* bishtbhawna4 AT gmail.com

The study describes an innovation in the area of low cost POC diagnostics enabling rapid detection of pathogens and diseases biomarkers by visible color change reaction in less than 15 minutes. The assay offers a new way of performing low-cost diagnostics, providing fewer operational steps, higher sensitivity, and easy interpretation of results in marked contrast to the most widely used lateral flow test cards, which offer only qualitative detection and require more biological reagents. The concept is based on enzyme-nanoparticles interaction and extends to the development of color shift test. At the centre-stage of the developed test is a nanoparticle that has the co-presence of a receptor and the inhibitor for an enzyme on its surface and both of these are properly displayed and nicely oriented to bind the target molecule that may be present in the solution. If interaction with the target occurs the inhibitor is no longer able to inhibit the enzyme that moves freely in solution and consequently its activity changes the color of the solution. The assay employs the good old basic science of enzyme amplification that converts a nanoscopic antigen-antibody reaction into a bulk phenomenon, i.e., a naked eye observable change in color. The utility of the test was also explored in environmental side for pathogen sensing [1] and for clinical application to detect Typhoid [2] and Cardiac biomarkers [3] in clinical sample (patient serum) by functionalizing the nanoparticle with respective affinity molecules. The color change is also quantifiable to give an exact analysis of the target using spectrophotometric or CCD mobile phone-based detection methods that can be operated very well by an end user. Validation with real samples demonstrated high specificity and sensitivity. The distinct color shift from yellow to pink provides an intuitive, equipment-free readout. This low-cost, rapid, and field-deployable immunoassay has significant potential to improve diagnostics, particularly in resource-limited settings.

---

**KEYWORDS:** Silver nanoparticles, Bifunctionalization, Color-shift, Biomarkers, Biosensing

---

**ACKNOWLEDGEMENTS:** Indian Council of Medical Research (ICMR), India CSIR-Institute of Microbial Technology (IMTECH), Chandigarh, India, 160036

---

### REFERENCES

- [1] V Kumar, A Chopra, B Bisht, V Bhalla. “Colorimetric and electrochemical detection of pathogens in water using silver ions as a unique probe”. *Scientific Reports*, 10, 11986 (2020)
- [2] B Bisht\*, M Choudhary\*, J K Saini, Bharti, P Singh, P Bhardwaj, R Dilawari, A K Pinnaka, P Ray, M Gupta, S Sethi, C. R Suri, M Raje and V Bhalla. “Bifunctionalized nanobioprobe-based rapid color-shift assay for Typhoid targeting Vi capsular polysaccharide”. *Biosensors and Bioelectronics*, 228, 115195 (2023)
- [3] Bharti; P. Bhardwaj; B. Bisht; Sagrika; R. Bala; M. Rohit; J. Singh; V. Bhalla, “Target-Induced shielding layer at dual-affinity probe interface for rapid colorimetric detection of cardiac biomarkers”. *ACS Applied material and interfaces*, 18, 8, 12423-12431 (2026)

## Excitation-dependent luminescence as a tool for probing site redistribution in $\text{Eu}^{3+}$ -doped silicate hydroxyapatite-type materials

N. Charczuk<sup>1</sup>\*, A. Watras<sup>1</sup>, R. Wiglusz<sup>1</sup>

*1) Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Poland*

\* n.charczuk AT intibs.pl

Nanosized hydroxyapatite-type materials (HAp) doped with  $\text{Eu}^{3+}$  ions represent a versatile group of luminescent materials, combining the red emission of trivalent europium ions with the biocompatibility of the hydroxyapatite matrix. A defining structural feature of the HAp lattice is the presence of two non-equivalent calcium positions—the  $C_3$ -symmetric Ca(1) and  $C_5$ -symmetric Ca(2) sites—both of which can be substituted by  $\text{Eu}^{3+}$  ions. While the general luminescence of HAp: $\text{Eu}^{3+}$  systems is well-documented, the use of site-selective excitation to probe specific crystallographic environments remains a less commonly utilized approach. Understanding the correlations between these local environments and the resulting optical response is key to designing bio-related materials with tailored properties.

In this work, we investigate silicate-substituted hydroxyapatite-type materials doped with  $\text{Eu}^{3+}$  ions (Si-HAp: $\text{Eu}^{3+}$ ), focusing on the relationship between excitation-dependent emission and structural changes arising from the incorporation of orthosilicate ions and thermal processing. A series of heat-treated materials, heated between 600 and 900 °C, was characterized using structural and spectroscopic techniques at room temperature and 6 K. The analysis clarifies the structural factors governing the observed luminescence and establishes a correlation between the local environment and optical response.

Using Si-HAp: $\text{Eu}^{3+}$  as a representative system, we outline a strategy for the rational design of hydroxyapatite-based materials with tunable, excitation-dependent properties. This approach provides a framework for applications such as optical tagging and can be extended to probing dopant distribution in other complex, multi-site inorganic systems.

---

**KEYWORDS:** Silicate-substituted hydroxyapatite-type materials,  $\text{Eu}^{3+}$ , Ion-doping, Excitation-dependent luminescence, Thermal treatment effects

---

**ACKNOWLEDGEMENTS:** We would like to acknowledge the National Science Centre, Poland (NCN) for financial support within the Project ‘Biocompatible materials with theranostics’ properties for precision medical application’ (No. UMO-2021/43/B/ST5/02960).

## Development and characterization of zinc oxide nanoparticles loaded pcl/cmc crosslinked composite films for enhanced in vitro wound healing applications

K. N. N. Prinindya<sup>1</sup>\*, S. M. A. Sadeq<sup>1</sup>, S. Mohsin<sup>1</sup>, M. Nawshad<sup>1</sup>, E. M. S. Ahmed<sup>1</sup>

1) Qatar University, Qatar

\* kn2401433 AT qu.edu.qa

### Abstract:

**Background:** Effective wound management remains a significant clinical challenge, particularly for chronic wounds that require a delicate balance of moisture maintenance, structural support, and robust protection against microbial infection [1]. Conventional dressings often fail to provide simultaneous antibacterial action and optimal mechanical properties, leading to delayed healing and increased risk of complications [2].

**Objective:** This study aims to address these requirements by developing and characterizing a novel composite film integrating Zinc Oxide (ZnO) nanoparticles into a crosslinked matrix of Polycaprolactone (PCL) and Carboxymethyl Cellulose (CMC).

**Methods:** The fabrication started with the crosslinking process of PCL and CMC using acetic acid, followed by the incorporation of ZnO nanoparticles into the resulting polymer solution. To ensure the homogeneous dispersion of the nanoparticles, the mixture was subjected to probe sonication prior to film casting [3]. The structural and chemical properties were evaluated using X-Ray Diffraction (XRD) and Fourier Transform Infrared Spectroscopy (FTIR). Thermal stability and phase transitions were tested using Thermogravimetric Analysis (TGA) and Differential Scanning Calorimetry (DSC). Physical properties were assessed via contact angle measurements and swelling tests, while the therapeutic potential was evaluated through in vitro antibacterial assays, nanoparticle release studies by ICP-MS and MTT assays to evaluate its biocompatibility [4].

**Results:** XRD and FTIR analyses confirmed successful polymer interaction and the uniform distribution of ZnO nanoparticles within the matrix. Contact angle measurements and swelling tests confirmed that the addition of CMC significantly enhanced the hydrophilicity of the composite film compared to pure PCL, providing a more suitable environment for cell migration. Furthermore, in vitro assays demonstrated potent antibacterial activity against *Staphylococcus aureus* and *Pseudomonas aeruginosa*, supported by a sustained release profile of the ZnO nanoparticles [5]. **Conclusion:** The results suggest that the ZnO-PCL-CMC crosslinked film is demonstrating significant potential in vitro as a highly effective candidate for treating chronic and infected wounds, offering a synergistic balance of mechanical strength, biocompatibility, and superior infection control.

---

**KEYWORDS:** Composite film, ZnO nanoparticles, Wound healing, Polycaprolactone, Carboxymethyl cellulose

---

**ACKNOWLEDGEMENTS:** This research was funded by Qatar National Research Fund, part of Qatar Foundation through the Academic Research Grant "ARG01-0531-230440".

### REFERENCES

- [1] E. Naseri and A. Ahmadi, "A review on wound dressings: Antimicrobial agents, biomaterials, fabrication techniques, and stimuli-responsive drug release," Jun. 15, 2022, Elsevier Ltd. doi: 10.1016/j.eurpolymj.2022.111293.
- [2] G. Pandey, T. Kolipaka, D. A. Srinivasarao, N. Abraham, A. Jain, and S. Srivastava, "Navigating the complexities of diabetic foot ulcers: From pathophysiology to advanced treatment strategies," *J. Drug Deliv. Sci. Technol.*, vol. 107, p. 106852, 2025, doi: <https://doi.org/10.1016/j.jddst.2025.106852>.
- [3] P. Guha Ray, R. Rajasekaran, B. Pratihari, S. De, S. Dhara, and M. Fussenegger, "Skin-Integrated Electro-genetic Regulation of Vasculature for Accelerated Wound Healing," *Adv. Sci.*, vol. 12, no. 9, Mar. 2025, doi: 10.1002/advs.202412257.
- [4] Y. Zhang *et al.*, "Ag nanocomposite hydrogels with immune and regenerative microenvironment regulation promote scarless healing of infected wounds," *J. Nanobiotechnology*, vol. 21, no. 1, Dec. 2023, doi: 10.1186/s12951-023-02209-2.
- [5] L. Siebert *et al.*, "Light-Controlled Growth Factors Release on Tetrapodal ZnO-Incorporated 3D-Printed Hydrogels for Developing Smart Wound Scaffold," *Adv. Funct. Mater.*, vol. 31, no. 22, May 2021, doi: 10.1002/adfm.202007555.

Posters

T11-10

E-POSTER

## The anticancer properties of metal nanocomposites obtained in xanthan and SiO<sub>2</sub>/polyacrylamide matrices: A comparative study

O. Akopova<sup>1\*</sup>, T. Zheltonozhskaya<sup>2</sup>, M. Tovstenko-Zabelin<sup>2</sup>, S. D. Zahorodnia<sup>3,4</sup>, V. Klepko<sup>2</sup>

1) Bogomoletz Institute of Physiology NAS of Ukraine, Ukraine

2) Institute of Macromolecular Chemistry, NAS of Ukraine, Ukraine

3) D.K. Zabolotny Institute of Microbiology and Virology of the National Academy of Sciences of Ukraine, Ukraine

4) D.K. Zabolotny Institute of Microbiology and Virology, NAS of Ukraine, Ukraine

\* olga-akopova AT biph.kiev.ua

Increasing multidrug resistance of tumors is a global health concern. Nanomedicine based on metal nanoparticles and metal nanocomposites is at the forefront of therapeutic strategies aimed at helping to resolve this problem. We aimed to examine the anticancer activity of metal nanocomposites obtained in chemically different polymer carriers: bacterial polysaccharide xanthan (X) and the polymer inorganic hybrid SiO<sub>2</sub>/grafted polyacrylamide (H). Methods: The water soluble nanocomposites with long lasting stability were synthesized in situ by NaBH<sub>4</sub> reduction and studied using XRD, UV Vis absorbance, FTIR, and TEM methods; their particle size, evaluated by TEM, was within the low nanoscale range of <10 nm. The anticancer activity was examined based on viability testing by the MTT test and the half inhibition concentrations IC<sub>50</sub>.

As shown, the systems could be separated into three groups with very high, high, and low activity, based on IC<sub>50</sub>. The dependence of anticancer efficacy on cell type, metal type, and matrix type was found. The Ag and Co systems, AgH, AgX, CoH, and CoX, exhibited very high activity against B<sub>95-8</sub> cells, with IC<sub>50</sub> of 1-6 µg/ml, close to that of anticancer drugs. Wish cells were highly sensitive to AgH, AgX, NiH, and CoH, with IC<sub>50</sub> of 7-10 µg/ml. AgH and CoX showed low activity for the control MDCK cells, with IC<sub>50</sub> of 15-20 µg/ml. NiX (IC<sub>50</sub> of 15-20 µg/ml) was the least active against any cell type. Among the cells, the most sensitive were B<sub>95-8</sub>, and the least sensitive were MDCK cells, according to the order: MDCK<Wish<B<sub>95-8</sub>. As we found, the metal activity was critically dependent on the carrier type. Xanthan greatly strengthened the effects of Ag against B<sub>95-8</sub> and MDCK cells, but dramatically reduced Ni toxicity for all cell types and Co toxicity against Wish cells. By itself, xanthan was not toxic to any cell type; however, it highly improved Ag efficacy against B<sub>95-8</sub> cells and dramatically weakened Ni efficacy against all studied cells. The effects of Co in the xanthan carrier were dependent on cell type. We assumed possible synergism of Ag and xanthan actions in B<sub>95-8</sub> cells and antagonism of Ni and xanthan actions in all studied cells.

Based on the experiments, we concluded that in situ synthesis of metal nanocomposites allowed the obtaining of metal nanoparticles in the low nanometer range with high anticancer activity and promise for oncomedicine. The carrier was critical for nanocomposite activity and was capable of either potentiating or abolishing the anticancer effects, while being nontoxic to the cells. The dependence of the observed effects on metal type, cell type, and carrier, and the underlying mechanisms, require detailed studies in future research.

**KEYWORDS:** Metal nanocomposites, Anticancer activity, Silver and cobalt nanoparticles, Xanthan and SiO<sub>2</sub>/polyacrylamide matrices, Cytotoxicity (IC<sub>50</sub>)

## Evaluation of the effect of protein adsorption on the mechanical bactericidal activity of nanostructured surfaces

T. Ito<sup>1\*</sup>, Y. Kamimura<sup>1</sup>, T. Shimizu<sup>1</sup>

1) Kansai University, Japan

\* t.ito AT kansai-u.ac.jp

Nanostructured surfaces inspired by cicada wings are known to exhibit bactericidal activity and have attracted attention as novel antimicrobial materials that do not rely on chemical agents. This bactericidal effect is reported to persist semi-permanently as long as the nanostructure remains intact and does not affect human cells, making such surfaces promising candidates for surface modification of medical devices that come into direct contact with the human body. However, under practical biomedical conditions, these surfaces may be exposed to blood and bodily fluids, which may potentially inactivate their bactericidal function. Despite this concern, there have been few studies investigating whether the bactericidal effect is maintained after the adsorption of biological components such as proteins, and this issue remains unclear. In this study, we quantitatively investigated the effect of protein adsorption on the physicochemical property and bactericidal activity of nanostructured surfaces, with the aim of clarifying how protein contamination influences their water contact angles and mechanical bactericidal performance.

In summary, protein (BSA) adsorption markedly altered surface wettability and led to a concentration-dependent reduction in bactericidal activity. Although bactericidal performance was diminished under protein-rich conditions, it was not completely lost, indicating partial retention of mechanical bactericidal functionality. These findings highlight protein adsorption as a critical challenge for the practical application of nanostructured bactericidal surfaces in biomedical devices and suggest that strategies to suppress protein adsorption will be essential for maintaining bactericidal performance in biological environments.

---

**KEYWORDS:** Mechano-bactericidal surfaces, Protein adsorption, Nanostructured surfaces, Antibacterial coatings

---

**ACKNOWLEDGEMENTS:** This research was conducted in part using the ORDIST HRC cleanroom at Kansai University.

---

### REFERENCES

- [1] E. P. Ivanova, J. Hasan, H. K. Webb, V. K. Truong, G. S. Watson, J. A. Watson, V. A. Baulin, S. Pogodin, J. Y. Wang, M. J. Tobin, C. Löbbe, R. J. Crawford, Natural bactericidal surfaces: Mechanical rupture of *Pseudomonas aeruginosa* cells by cicada wings, *Small*, Vol. 8, pp. 2489-2494, 2012.
- [2] A. Velic, J. Hasan, Z. Li, P. K. D. V. Yarlagadda, Mechanism of bactericidal interaction and death on nanopatterned surfaces, *Biophys. J.*, Vol. 120, pp. 217-231, 2021.
- [3] J. Jenkins, J. Mantell, C. Neal, A. Gholinia, P. Verkade, A. H. Nobbs, B. Su, Antibacterial effects of nanopillar surfaces are mediated by cell impedance, penetration and induction of oxidative stress, *Nat. Commun.*, Vol.11, 1626, 2020.
- [4] S. Mimura, T. Shimizu, S. Shingubara, H. Iwaki, T. Ito, Bactericidal effect of nanostructures via lytic transglycosylases of *Escherichia coli*, *RSC Adv.*, Vol. 12, pp. 1645-1652, 2022.
- [5] N. Lin, P. Berton, C. Moraes, R. D. Rogers, N. Tufenkij, Nanodarts, nanoblades, and nanospikes: Mechano-bactericidal nanostructures and where to find them, *Adv. Colloid Interface Sci.*, Vol. 252, pp. 55-68, 2018.
- [6] K. Minoura, M. Yamada, T. Minogushi, T. Kaneko, K. Nishiyama, M. Ozminsky, T. Koshizuka, I. Wada, T. Suzutani, Antibacterial effects of the artificial surface of nanoimprinted moth-eye film, *Plos One*, 018366, 2017.
- [7] A. R. Collaborators, Global burden of bacterial antimicrobial resistance in 2019: A systematic analysis, *Lancet*, Vol 399, pp. 629-655, 2022.
- [8] T. Ito, Y. Yanagisawa, G. Yamamoto, S. Hamagushi, S. Kustsuna, T. Shimizu, S. Shingubara, Antibacterial Property of Si Nanopillars for Anti-Microbial Resistance (AMR) Bacteria, *J. Photopolymer Sci. Tech.*, Vol. 38, pp.85-90, 2025.
- [9] H. Masuda, K. Fukuda, Ordered metal nanohole arrays made by a two-step replication of honeycomb structures of anodic alumina, *Science*, Vol. 268, pp. 1466-1468, 1995.
- [10] N. Ogawa, K. Sato, K. Sunada, H. Ishiguro, H. Kojima, T. Ito, Polymeric antibacterial surfaces with nano-pillar arrays mimicking cicada wings, *J. Photopolymer. Sci. Tech.*, Vol. 35, pp. 213-216, 2022.

## Sodium citrate potentiated degradation of HepG<sub>2</sub> spheroids by supramolecular nanocomplexes and pharmacological ascorbic acid

G. Dudetskaya<sup>1\*</sup>, V. Seminko<sup>1</sup>, P. Maksimchuk<sup>1</sup>, Y. Kot<sup>2</sup>, V. Klochkov<sup>1</sup>, O. Sedyh<sup>1</sup>

1) Institute for Scintillation Materials, NAS of Ukraine, Ukraine

2) V. N. Karazin Kharkiv National University, Ministry of Education and Science of Ukraine, Kharkiv, Ukraine, Ukraine

\* gdudetska AT gmail.com

The use of sodium citrate (SCT) to potentiate the antitumor activity of therapeutic agents has attracted increasing attention in recent years. The underlying mechanism is believed to involve enhanced intracellular transport in tumor cells and reduced density of tumor structures.

In the present study, we evaluated the capacity of citrate to augment the cytotoxic efficacy of supramolecular complexes based on orthovanadates or nanoceria and containing menadione (or polyphenols as an alternative quinone source) when combined with pharmacological concentrations of ascorbic acid (AA). The synergistic interaction between AA and nanoceria-based complexes that produces a pan-killing effect had previously been confirmed in both 2D and 3D models of murine L<sub>929</sub> fibrosarcoma. In the current experiments, this synergy was successfully reproduced in long-term monolayer cultures of HepG<sub>2</sub> cells. However, the 3D HepG<sub>2</sub> spheroid model demonstrated substantially higher resistance to treatment than L<sub>929</sub> spheroids, owing to the markedly greater structural density of HepG<sub>2</sub> aggregates.

To disrupt the compact intercellular architecture maintained by CaZ<sup>+</sup> ions, citrate was introduced as a specific CaZ<sup>+</sup> chelator. Careful selection of effective citrate concentrations resulted in loosening of the spheroid matrix, followed by progressive degradation during prolonged co-incubation with the nanocomplexes and ascorbic acid.

Furthermore, extended exposure to the citrate-ascorbic acid-nanoparticle system in combination with polyphenols similarly induced HepG<sub>2</sub> spheroid degradation, accompanied by sustained cytotoxic activity thereafter.

---

**KEYWORDS:** Sodium citrate, Supramolecular complexes, Ascorbic acid, Polyphenols, Spheroid

---

**ACKNOWLEDGEMENTS:** This research was supported by National Research Foundation of Ukraine, Grant № 2023.03/0050.

## Synergistic photoprotective effects of carbon-cerium dioxide nanocomposites on mouse bone marrow cells under UV-a irradiation

V. Sarnatskaya<sup>1\*</sup>, P. Virych<sup>2</sup>, Y. Shlapa<sup>3</sup>, L. Paziuk<sup>4</sup>, V. Mikhailenko<sup>1</sup>, K. Saulenko<sup>5</sup>, A. Bilous<sup>3</sup>

1) R. e. Kavetsky Institute of Experimental Pathology, Oncology and Radiobiology of the NAS of Ukraine, Ukraine

2) Chemical Faculty, Taras Shevchenko National University of Kyiv, Ukraine

3) V. Vernadsky Institute of General and Inorganic Chemistry, NAS of Ukraine, Ukraine

4) Educational-scientific Centre "Institute of Biology and Medicine", Taras Shevchenko National University of Kyiv, Ukraine

5) RE Kavetsky Institute of Experimental Pathology, Oncology and Radiobiology, National Academy of Sciences of Ukraine, Ukraine

\* vsnikavera AT gmail.com

Ultraviolet (UV) irradiation is a cornerstone of photoactivated biomedical technologies; however, it inevitably induces oxidative stress via the generation of intracellular reactive oxygen species (ROS). This results in dose-dependent morphological alterations, metabolic shifts, and diminished cell viability. Consequently, understanding how nanomaterials modulate cellular responses under UV-A exposure is essential for engineering biocompatible, light-responsive systems. This study investigates the photobiological impacts of carbon particles (CPs), cerium dioxide nanoparticles (CeO<sub>2</sub> NPs), and hybrid carbon-cerium dioxide nanocomposites (C-CeO<sub>2</sub> NCs) on mouse bone marrow cells (MBMCs) under controlled 390 nm UV- A irradiation. Our results demonstrate that CPs exhibit concentration-dependent cytotoxicity, with exacerbated phototoxicity at high concentrations, yet significant ROS reduction at lower doses. Conversely, CeO<sub>2</sub> NPs show minimal intrinsic toxicity and robust antioxidant activity, effectively attenuating UV-induced oxidative stress. Notably, the C-CeO<sub>2</sub> NCs exhibit a balanced biological response, integrating the antioxidant properties of ceria with the radical-scavenging and electron-transfer capabilities of carbon to preserve cellular structural integrity. Comprehensive morphological, morphometric, and immunocytochemical analyses of key regulatory markers (p53, p21, Bcl-2, E-cadherin,  $\beta$ -catenin, and Ki-67) reveal that the nanocomposite composition modulates interconnected pathways governing MBMC proliferation, survival, and adhesion.

These findings highlight the potential of carbon-ceria nanostructures as redox-active biomaterials for applications requiring precise photomodulation and cellular protection against photodamage.

Potential fields of application include skin tissue engineering, light-exposed implants, photodynamic therapy, ophthalmic systems, light-responsive drug delivery systems, regenerative medicine, and advanced dermatological formulations.

---

**KEYWORDS:** Nanocomposites, Ultraviolet, Photoprotective effects

---

**ACKNOWLEDGEMENTS:** This work was supported by the National Research Foundation of Ukraine under grant No 86.07/0032.

## Eco-friendly nanocomposite films based on chitosan and alginate incorporating green-synthesized wild thymus-mediated AgNPs for biomedical and food applications

A. Nicolae-Maranciuc<sup>1\*</sup>, G. Bucher<sup>2</sup>, J. Ponti<sup>2</sup>, H. El Hadri<sup>2</sup>, G. Schirinzi<sup>2</sup>, A. Valsesia<sup>2</sup>

1) Institute for Interdisciplinary Studies and Research (ISCI), Lucian Blaga University of Sibiu; Research Center for Complex Physical Systems, Faculty of Sciences, Lucian Blaga University of Sibiu, Romania

2) European Commission, Joint Research Centre, Ispra, Italy

\* alexandra.nicolae AT ulbsibiu.ro

The development of sustainable eco-friendly antimicrobial thin films and membranes is crucial for the evolution of biomedical and food applications while minimizing environmental impact. In this study, thin polymeric membranes based on chitosan and sodium alginate were fabricated and reinforced with green-synthesized silver nanoparticles (AgNPs). The AgNPs were obtained via an eco-friendly biosynthesis route using aqueous extracts of *Wild Thymus* species from Romania as both reducing and stabilizing agents. The resulting nanoparticles exhibited uniform size distribution and strong surface plasmon resonance, confirming successful synthesis through UV-VIS, TEM, FT-IR and ICP-MS analysis. Also, FT-IR results showed differences between the plant extract and the green synthesized AgNPs proving the involvement of the phytochemicals from plants in the metallic ions reductions. Incorporation of the green-synthesized AgNPs into the chitosan-alginate matrix enhanced the membranes' mechanical stability, barrier properties, and antimicrobial activity against common foodborne pathogens such as *Escherichia coli* and *Staphylococcus aureus*. The biopolymer-based membranes demonstrated excellent transparency, flexibility, and biodegradability, while the integration of AgNPs was confirmed by TEM-EDX analysis. This work highlights the potential of combining natural polymers with plant-mediated silver nanoparticles to produce environmentally friendly, functional biomedical/packaging antibacterial materials that align with circular economy principles.

---

**KEYWORDS:** Silver nanoparticles, Green chemistry, Membrane, Chitosan, Biomedical and food applications

---

**ACKNOWLEDGEMENTS:** Project financed by Lucian Blaga University of Sibiu through the research grant LBUS-IRG-2024.

## Biological potential of 3d printing for bone-replacing implants

A. Bakalo<sup>1</sup>\*, Y. Kuzenko<sup>1</sup>, M. Skydanenko<sup>1</sup>, Ponomarova<sup>1</sup>, A. Kovchun<sup>1</sup>, I. Makhnyuk<sup>1</sup>

1) Sumy State University, Ukraine

\* anyabakalo AT gmail.com

The regeneration of critical bone defects resulting from trauma, oncological resections, or systemic diseases remains a significant clinical challenge due to the limitations of traditional autografting. Modern three-dimensional (3D) bioprinting technology enables the fabrication of customized scaffolds with precise anatomical geometry by combining biopolymers and bioactive inorganic phases. [1, 2] However, the development of biomaterials capable of accurately mimicking the natural extracellular matrix of bone - while providing appropriate mechanical properties and biological cues for regeneration - remains an unresolved issue. Here we show that photochemical crosslinking using riboflavin, combined with the integration of hydroxyapatite, allows for the formation of structurally stable biomimetic collagen matrices. [3] We found that upon UV irradiation, riboflavin initiates the formation of intermolecular covalent bonds within collagen, which increases mechanical integrity and elastic modulus while preserving the native fibrillar architecture of the material. Furthermore, the adaptation of the FRESH methodology in combination with physicochemical stimuli (vacuum degassing, moderate pressure, and controlled thermal modulation) ensured the formation of a composite with a hierarchically organized microstructure. These structural features are critically important for facilitating nutrient transport, cellular infiltration, and effective tissue integration in vivo. [4] We anticipate this approach to be a robust foundation for the development of advanced osteoconductive and osteoinductive biomaterials. Ultimately, the application of such optimized 3D-bioprinted implants holds significant potential for improving clinical outcomes in regenerative medicine and bone tissue engineering.

---

**KEYWORDS:** 3D bioprinting, Bone tissue engineering, Collagen-hydroxyapatite composites, Photochemical crosslinking, Regenerative medicine

---

### REFERENCES

- [1] M. Meyer, Processing of collagen based biomaterials and the resulting materials properties. *BioMedical Engineering OnLine* (2019).
- [2] T.M. Koushik, C.M. Miller, E. Antunes, Bone Tissue Engineering Scaffolds: Function of Multi-Material Hierarchically Structured Scaffolds. *Advanced Healthcare Materials*, 12, 2202766 (2023).
- [3] Y. Koo, G.H. Kim, Bioprinted hASC-laden collagen/HA constructs with meringue-like macro/micropores. *Bioengineering & Translational Medicine*, 7, e10330 (2022).
- [4] S.P. Moss, D.J. Shiwerski, A.W. Feinberg, FRESH 3D Bioprinting of Collagen Types I, II, and III. *ACS Biomaterials Science & Engineering*, 11, 556-563 (2025).

## Antioxidant and hemostatic chitosan nanocomposite films modified with quercetin, graphene oxide and microcrystalline cellulose: In vitro biocompatibility assessment

B. Bielska<sup>1</sup>\*, A. El Kadib<sup>2</sup>, K. Miłowska<sup>3</sup>

1) Department of General Biophysics, Faculty of Biology and Environmental Protection, University of Lodz, University of Lodz Doctoral School of Exact and Natural Sciences, University of Lodz, Lodz, Poland, Poland

2) Euromed Research Center, Engineering Division, Euro-Med University of Fes (UEMF), Fès 30070, Morocco, Morocco

3) Department of General Biophysics, Faculty of Biology and Environmental Protection, University of Lodz, Poland

\* beata.bielska AT edu.uni.lodz.pl

Natural polymer-based films have attracted considerable attention as biomedical coating materials due to their favorable biological and mechanical properties. Among them, chitosan films have been widely investigated as coating platforms and as wound-healing dressings. In the context of wound repair, polyphenol-modified, chitosan-based composites can further enhance antimicrobial, antioxidant, and regenerative responses, thereby accelerating tissue regeneration [1].

The aim of this study was to assess the toxicity of chitosan-based nanocomposites modified with varying concentrations of quercetin, as well as with graphene oxide and microcrystalline cellulose, towards human erythrocytes, skin fibroblast cell lines, and peripheral blood mononuclear cells (PBMCs), using both direct and indirect contact between the material and the biological models. Furthermore, the protective properties of the composites were assessed using a hydrogen peroxide-induced oxidative stress model. The hemostatic potential of the chitosan films, including their effects on blood clotting and clot dissolution, was also examined.

The results demonstrated that the chitosan films exhibited minimal hemolytic activity toward erythrocytes, at approximately 5%. A similar trend was observed in the context of cellular viability studies, wherein the films exhibited a marginal reduction in cell viability, ranging from 10 to 15%, across all the variants examined. The presence of quercetin resulted in an enhancement of the antioxidant properties of the films, as evidenced by the oxidative stress model. In addition, the chitosan films exhibited hemostatic properties by modulating blood clotting and promoting clot dissolution. These findings suggest that chitosan-based films have potential for use in hemostatic applications and justify further investigation in wound-healing systems. Furthermore, the combination of chitosan with bioactive compounds may yield novel beneficial effects or augment existing ones, thereby optimising patient outcomes and reducing healthcare expenditures.

---

**KEYWORDS:** Chitosan nanocomposites, Quercetin-modified chitosan, Graphene oxide, Microcrystalline cellulose, Wound healing

---

### REFERENCES

- [1] B. Bielska & K. Miłowska, “Therapeutic potential of chitosan-based and related nanocomposite systems in wound management: A review”, *International Journal of Molecular Sciences*, 26(23), 11748, (2025).

## Activated carbon particles promote mitochondrial dysfunction and apoptosis under nitrosative stress in vitro

V. Mikhailenko<sup>1\*</sup>, A. Glavin<sup>2</sup>, P. Virych<sup>3</sup>, V. Sarnatskaya<sup>1</sup>

1) R. e. Kavetsky Institute of Experimental Pathology, Oncology and Radiobiology of the NAS of Ukraine, Ukraine

2) R.E. Kavetsky Institute of Experimental Pathology, Oncology and Radiobiology NASU, Ukraine

3) Chemical Faculty, Taras Shevchenko National University of Kyiv, Ukraine

\* mvmik AT yahoo.com

Dietary and environmental exposure to inorganic nitrates ( $\text{NO}_3^-$ ) and nitrites ( $\text{NO}_2^-$ ) significantly disrupts redox homeostasis, promoting oxidative and nitrosative stress. This induces lipid peroxidation, protein tyrosine nitration, and S-nitrosylation of thiol groups, resulting in mitochondrial dysfunction ultimately leading to apoptosis or necrosis depending on exposure severity. In this context, activated carbon particles (ACP) represent a promising nanobiotechnological strategy for mitigating  $\text{NO}_2^-/\text{NO}_3^-$ -induced toxicity due to their high surface area and redox-modulating properties.

The study investigates the effects of ACP on mouse aortic endothelial cells (MAEC) treated with  $\text{IC}_{50}$  doses of  $\text{NO}_2^-$  or  $\text{NO}_3^-$ . The results show that the addition of ACP to the MAEC culture medium increased mitochondrial transmembrane potential (MTP) by 2.1-fold and reactive oxygen species (ROS) production by 2.3-fold. Apoptosis and necrosis were assessed by multiparametric flow cytometry using Annexin V and 7-aminoactinomycin D. Early apoptosis increased from a spontaneous level of 4.7% to 20.4% following ACP treatment. Exposure to  $\text{NO}_2^-$  and  $\text{NO}_3^-$  alone increased MTP by 2.3- and 2.1-fold, respectively, while ROS production increased by 1.5- and 1.8-fold. Apoptosis levels also rose by 3.8- and 3.0-fold compared to intact cells. Combined treatment with ACP and  $\text{NO}_2^-$  or  $\text{NO}_3^-$  showed no additive effects on MTP or ROS production. MTP increased by 2.1-2.2-fold and ROS by 1.7-2.0-fold relative to intact cells. However, combined exposure further elevated apoptosis by 1.5-2.6-fold compared to ACP treatment alone. Notably, necrosis and late-stage apoptosis remained minimal ( $\leq 0.43\%$ ) across all experimental groups, indicating that  $\text{NO}_2^-/\text{NO}_3^-$  primarily act via regulatory signaling rather than direct cytotoxicity.

Overall, our results suggest that both  $\text{NO}_2^-/\text{NO}_3^-$  and ACP significantly affect cellular stress responses, including mitochondrial function and redox balance, while combined exposure does not confer protective effects and instead enhances apoptosis. Furthermore, these findings indicate that engineered nanomaterials can modulate key stress-response pathways and thereby influence cell fate under environmental exposure conditions.

**KEYWORDS:** Inorganic nitrates and nitrites, Reactive oxygen species, Mitochondrial transmembrane potential, Apoptosis

## UV-activated (Gd,Y)VO<sub>4</sub>:Eu<sup>3+</sup> nanocrystals as sources of oxygen-independent ROS after external stimuli removal

P. Maksimchuk<sup>1\*</sup>, O. Ivanov<sup>1</sup>, V. Seminko<sup>1</sup>, M. Lupan<sup>1</sup>, G. Grygorova<sup>1</sup>, O. Samoilo<sup>1</sup>, A. Onishchenko<sup>2</sup>, V. Klochkov<sup>1</sup>, S. Yefimova<sup>1</sup>

1) Institute for Scintillation Materials, NAS of Ukraine, Ukraine

2) Kharkiv National University of Radio Electronics, Ukraine

\* pavel.maksimchuk AT gmail.com

The hypoxic microenvironment in solid tumors largely contributes to the failure of PDT in most tumor treatments [1]. Classical PDT relies heavily on the presence of dissolved oxygen to generate cytotoxic singlet oxygen (<sup>1</sup>O<sub>2</sub>), which makes this method inherently ineffective in oxygen-deprived regions of a tumor [2]. To overcome these fundamental constraints, we developed defect-engineered (Gd,Y)VO<sub>4</sub>:Eu<sup>3+</sup> nanocrystals (NCs), that can produce radical species such as •OH through water oxidation after UV pre-irradiation.

These orthovanadate NCs are characterized by a high density of oxygen vacancies [3], that act as metastable traps for photo-generated holes created during UV pre-irradiation. The charge carried by the holes that are trapped does not recombine quickly. Rather, holes escape slowly and are mainly dictated by the process of moving to the particle surface by diffusion. Once reaching the particle surface, the trapped carriers eventually react (after a relatively long period of time since the light has turned off) with a water molecule to produce •OH. Unlike conventional photosensitizers, these NCs facilitate the production of •OH directly from water molecules, ensuring a robust, oxygen-independent cytotoxic mechanism. This unique "memory effect" allows for the sustained generation of radicals long after the initial light stimulus has been removed, providing a sophisticated strategy for treating malignant cells in hypoxic environments where traditional modalities fail.

The pro-oxidative activities of UV-activated (Gd,Y)VO<sub>4</sub>:Eu<sup>3+</sup> NCs were confirmed through several methods, which employed luminescence spectroscopy to monitor the conversion of a coumarin probe into fluorescent 7-hydroxycoumarin as a direct indicator of sustained •OH production. This robust oxidative capacity in aqueous environments was further highlighted by tracking the accelerated oxidation of ascorbic acid, which showed a significant loss and depletion in the presence of the pre-irradiated NCs. Finally, lipid oxidation analysis of phosphatidylcholine suspensions demonstrated significant oxidative damage through the formation of conjugated dienes, further validating the ability of the activated NCs to trigger radical chain reactions.

The defect-engineered NCs can produce efficient radicals independent of the continuous light supply and dissolved oxygen and therefore allow the creation of highly innovative strategies to treat malignant tissues within hypoxic environments that have always represented the fundamental limitations associated with the classical methodology of PDT.

---

**KEYWORDS:** Pro-oxidative activity, OH radical, Orthovanadate nanocrystal, UV pre-irradiation

---

**ACKNOWLEDGEMENTS:** This research was supported by National Research Foundation of Ukraine, Grant № 2025.07/0093

### REFERENCES

- [1] M. Valko, D. Leibfritz, J. Moncol, M. T. Cronin, M. Mazur, J. Telser, "Free radicals and antioxidants in normal physiological functions and human disease", *Int. J. Biochem. Cell Biol.*, 39, 44 (2007).
- [2] L. Tong, C. C. Chuang, S. Wu, L. Zuo, "Reactive Oxygen Species in Redox Cancer Therapy", *Cancer Letters*, 367, 18 (2015).
- [3] P. O. Maksimchuk, K. O. Hubenko, V. V. Seminko, V. L. Karbivskii, A. S. Tkachenko, A. I. Onishchenko, V. Yu. Prokopyuk, S. L. Yefimova, "High antioxidant activity of gadolinium-yttrium orthovanadate nanoparticles in cell-free and biological milieu", *Nanotechnology*, 33, 055701 (2022).

## Dual control of pro-oxidant behavior in nanoceria via iron doping and facet engineering

M. Lupan<sup>1</sup>\*, P. Maksimchuk<sup>1</sup>, V. Seminko<sup>1</sup>, G. Grygorova<sup>1</sup>, S. Yefimova<sup>1</sup>

1) Institute for Scintillation Materials, NAS of Ukraine, Ukraine

\* nikita.lupan4 AT gmail.com

For over two decades, cerium oxide nanocrystals (nanoceria) have been studied predominantly as antioxidants. Recent efforts, however, have shifted toward exploiting their pH-triggered pro-oxidant activity for applications in oncology, antimicrobials, and catalysis[1]. A major challenge in this field is the inefficient transition from scavenging to generating reactive oxygen species (ROS) at acidic pH. This study investigates how iron ( $\text{Fe}^{3+}$ ) doping and morphology engineering can be used to accelerate this transition and maximize catalytic output.

Our data reveal that  $\text{Fe}^{3+}$  incorporation increases peroxidase-like activity by facilitating oxygen vacancy formation through charge compensation. This effect follows a non-linear trend, reaching a maximum at 5% doping—a threshold that significantly surpasses the performance of both 3% and 10% concentrations. Furthermore, the activity is strongly dictated by the exposed crystallographic facets. Cubic nanocrystals, characterized by {100} planes, demonstrate 7-8 times higher efficiency than {111}-terminated octahedra, a result of lower defect formation energies on the cubic surface.

Kinetic analysis further reveals a fundamental divergence in the reaction pathways: {100} facets operate via a Ping-Pong mechanism, while {111} facets follow a sequential model. This distinction suggests that the interaction with hydrogen peroxide ( $\text{H}_2\text{O}_2$ ) is facet-specific. The Ping-Pong pathway on {100} planes indicates a radical-based process, where  $\text{H}_2\text{O}_2$  first dissociates into hydroxyl radicals ( $\cdot\text{OH}$ ) before substrate oxidation occurs. Conversely, the sequential mechanism on {111} planes implies a ternary complex formation, where  $\text{H}_2\text{O}_2$  and the substrate (e.g., TMB) must be co-adsorbed for electron transfer to take place. These insights provide a precise strategy for tailoring the redox behavior of nanoceria, facilitating the development of more effective pro-oxidant therapeutic agents.

---

**KEYWORDS:** Ceria, Doping, Prooxidant, Morphology

---

**ACKNOWLEDGEMENTS:** This research was supported by National Research Foundation of Ukraine, Grant № 2025.07/0093.

---

### REFERENCES

- [1] A. Datta, S. Mishra, K. Manna, K.D. Saha, S. Mukherjee, S. Roy. Pro-Oxidant Therapeutic Activities of Cerium Oxide Nanoparticles in Colorectal Carcinoma Cells ACS Omega 5 (2020) 9714.

## Polymeric cryogel materials for regeneration of living tissues and wound healing

V. Demchenko<sup>1\*</sup>, O. Demchenko<sup>2</sup>, S. Rushkovsky<sup>3</sup>, N. Rybalchenko<sup>4</sup>, O. Buryanov<sup>5</sup>

1) E.O. Paton Electric Welding Institute of the National Academy of Sciences of Ukraine, Ukraine

2) National Research Center for Radiation Medicine, the National Academy of Medical Sciences of Ukraine, Ukraine

3) Taras Shevchenko National University of Kyiv, Ukraine

4) D.K. Zabolotny Institute of Microbiology and Virology of the National Academy of Sciences of Ukraine, Ukraine

5) Bogomolets National Medical University, Ukraine

\* dvaleriy1 AT ukr.net

Currently, a relevant idea is the creation and study of polymer cryogels with effective antimicrobial action, which can be used for regeneration of living tissues and wound healing.

A series of polymer cryogel samples based on polyvinyl alcohol (PVA) with different contents of polyglutamic acid (PGA) (3, 5, 9 wt.%) and different concentrations of Ag<sub>2</sub>O nanoparticles (0.01, 0.05, 0.1, 0.5, 1.0 wt.%) were created for regeneration of living tissues and wound healing. After synthesis, the samples were poured into polypropylene bags measuring 10×10 cm, sealed and sterilized in an autoclave at a temperature of 120 °C for 20 min. At the next stage, the samples were crosslinked by freezing/thawing for different times at a temperature of (-20 °C). The optimal time for the formation of crosslinked cryogels was established: for PVA-PGA-Ag<sub>2</sub>O it was 150 min.

The synthesized series of cryogel materials were characterized by a complex of modern structural-morphological, physicochemical and physicomechanical methods. The water absorption of the samples was studied.

It was found that polyglutamic acid in the polymer matrix acted as a reducing agent for silver nitrate salts and a stabilizer of nanoparticles.

Studies of the created cryogel materials were conducted on a wide range of different microorganisms. In particular, the created materials were tested against opportunistic microorganisms, including gram-positive (*S. aureus*, *S. epidermidis*) and gram-negative (*E. coli*, *P. aeruginosa*) bacteria. The genotoxicity of the obtained samples was studied using the cytogenetic method and Comet Assay. The ability of the obtained materials to stimulate tissue regeneration was investigated on a model of fibroblast cell cultures. The level of wound healing was determined on a model of laboratory animals (rats) by macroscopic assessment, histological studies and determination of biochemical markers. As a result of comprehensive structural-morphological, physicochemical, physico-mechanical and biological studies, optimal conditions were identified for the formation of cryogel materials with effective bactericidal action, which do not exhibit cyto- and genotoxic effects and can be used for the regeneration of living tissues and wound healing: concentration of polyvinyl alcohol and polyglutamic acid, freezing temperature and time, optimal concentration of metal nanoparticles.

---

**KEYWORDS:** Cryogel, Polyglutamic acid, Wound surface

---

**ACKNOWLEDGEMENTS:** The work was carried out with financial support from the National Research Foundation of Ukraine grant "Development of biopolymer nanocomposite materials for stimulating the regeneration of living tissues and wound healing" (Application ID 2023.05/0009).

## Dual-affinity nanointerface for rapid translational detection of cardiac biomarkers via target-induced shielding mechanism

B. Bharti<sup>1</sup>\*, J. Singh<sup>1</sup>, V. Bhalla<sup>2</sup>

1) Department of Biotechnology, Panjab University, Chandigarh, India

2) CSIR-Institute of Microbial Technology Chandigarh India, India

\* bhartishiva1991 AT gmail.com

Rapid detection of cardiac biomarkers is critical for timely diagnosis and management of acute cardiovascular diseases, however conventional immunoassays often suffer from slow response, limited sensitivity, and low adaptability to point-of-care detection. Herein, we developed a colorimetric assay based on a target-induced shielding at a dual-affinity probe interface for detection of cardiac troponin I (cTnI) and N-terminal pro-B-type natriuretic peptide (NT-proBNP). Both biomarkers are clinically relevant gold standard biomarkers of acute myocardial infarction (AMI) and heart failure (HF) [1-2]. The assay leverages on dual-affinity probe that act as an inhibitor to the enzyme (urease) and have the co-presence on its surface of affinity molecules against biomarkers. Upon addition of target biomarker, the probe selectively binds to it and a shielding layer is formed that renders the enzyme free in solution. Consequently, the activity of enzyme generates a pink-colored endpoint for visual detection in <15 min. Comprehensive biophysical characterization using microscale thermophoresis (MST), bilayer interferometry (BLI), and isothermal titration calorimetry (ITC) confirmed strong target-probe interactions and elucidated the shielding mechanism. Importantly, the assay demonstrated negligible interference in complex biological matrices, maintaining analytical performance in MST up to 50% human serum [3]. The platform achieved a detection limit as low as 0.088 ng/mL for cTnI, with high specificity, reproducibility, and recovery in spiked serum. The robustness of assay highlights its translational potential for rapid, visual, and point-of-care cardiac diagnostics, offering a versatile framework adaptable to diverse protein biomarkers in nanobiomedical applications.

---

**KEYWORDS:** Dual-affinity probe, Colorimetric assay, Cardiac biomarkers, Point-of-care diagnostics, Probe shielding layer

---

**ACKNOWLEDGEMENTS:** The author thanks PU and CSIR for their facilities and support to enable this research. Author also thank ICMR for SRF fellowship.

---

### REFERENCES

- [1] X. Du, X. Su, W. Zhang, S. Yi, G. Zhang, S. Jiang, F. Xia, “Progress, opportunities, and challenges of troponin analysis in the early diagnosis of cardiovascular diseases”, *Analytical Chemistry*, 94, 442-463 (2021).
- [2] V. Panagopoulou, S. Deftereos, C. Kossyvakis, K. Raisakis, G. Giannopoulos, G. Bouras, M. W. Cleman, “NTproBNP: an important biomarker in cardiac diseases”, *Current topics in medicinal chemistry*, 13, 82-94 (2013).
- [3] Bharti; P. Bhardwaj; B. Bisht; R. Bala; Sagrika; M. Rohit; V. Bhalla, “Target-Induced Shielding Layer at the Dual-Affinity Probe Interface for Rapid Colorimetric Detection of Cardiac Biomarkers”, *ACS Applied Materials & Interfaces*, 18, 12423-12431 (2026).

## Mechanistic divergence in NADPH-quercetin-nanozyme systems: Surface-associated electron transfer in orthovanadates versus semiquinone-associated redox activity in nanoceria

N. Kavok<sup>1\*</sup>, V. Klochkov<sup>1</sup>, V. Seminko<sup>1</sup>, Y. Nikitchenko<sup>1</sup>, G. Dudetskaya<sup>1</sup>, O. Sedyh<sup>1</sup>

*1) Institute for Scintillation Materials, NAS of Ukraine, Ukraine*

\* yakavok AT gmail.com

Redox processes were investigated in model systems containing ultrasmall GdYVO<sub>4</sub>:Eu<sup>3+</sup> orthovanadate nanoparticles and nanoceria (CeO<sub>2</sub>, 2 nm) in the presence of NADPH and quercetin. Interest in such systems is driven by the growing relevance of artificial nanozymes capable of modulating redox homeostasis in biological environments. The ternary NADPH-quercetin-NP systems exhibited enhanced NADPH oxidation and evolution toward attenuated or quasi-stationary kinetic behavior at neutral and mildly acidic pH; however, the underlying mechanisms differed substantially between CeO<sub>2</sub> and orthovanadate nanoparticles. The results suggest that different mechanistic regimes operate in nanoceria- and orthovanadate-containing ternary NADPH-quercetin-nanoparticle systems. In the presence of nanoparticles and dissolved oxygen/peroxide, quercetin undergoes oxidation accompanied by formation of transient quercetin-derived redox intermediates, including semiquinone-like species, which may contribute to secondary electron-transfer reactions and reactive oxygen species generation. Short-time absorbance measurements demonstrated rapid activation of NADPH oxidation immediately after addition of quercetin, indicating efficient initial electron transfer in ternary systems. In contrast, longer fluorescence monitoring of NADPH over 10 min revealed progressive attenuation of the apparent oxidation rate following the initial activation phase. Thus, short-time kinetics mainly reflect rapid nanoparticle-mediated initiation processes, whereas longer fluorescence measurements characterize subsequent temporal stabilization of the redox system. The observed kinetic behavior did not demonstrate the progressive autoacceleration expected for sustained homogeneous semiquinone-driven redox cycling. Instead, the reactions exhibited an initial burst phase followed by attenuation or quasi-stationary behavior, suggesting an important contribution of interfacial and surface-associated electron-transfer processes. In nanoceria-containing systems, spectroscopic features were consistent with partial involvement of semiquinone-associated redox activity and transient quercetin-derived intermediates with partial diffusible character. In contrast, orthovanadate nanoparticles predominantly promoted coordination-mediated and surface-associated electron transfer without convincing evidence for self-sustaining bulk redox cycling. Thus, the data support coexistence of two distinct nanozyme-polyphenol interaction regimes: (i) semiquinone-associated redox activity with partial diffusible character in CeO<sub>2</sub> systems, and (ii) predominantly interfacial electron transfer in orthovanadate systems. These findings provide mechanistic insight into nanozyme-polyphenol interactions and demonstrate that nanoparticle composition critically determines the balance between surface-associated and diffusible redox pathways.

**KEYWORDS:** GdYVO<sub>4</sub>/Eu<sup>3+</sup> nanoparticles, NADPH, Interfacial electron transfer, Semiquinone intermediates, Redox activity

## Biocompatible red emitting fluorinated carbon dots: Synthesis, optical properties and fluorescent cell imaging

V. Skryshevsky<sup>1</sup>\*, I. Lysenko<sup>1</sup>, A. Topchylo<sup>2</sup>, A. Zaderko<sup>3</sup>, O. Pylypova<sup>4</sup>, A. Geloën<sup>5</sup>, N. Dziubenko<sup>1</sup>,  
H. Kuznietsova<sup>1</sup>, V. Lysenko<sup>3</sup>

1) Taras Shevchenko National University of Kyiv, Ukraine

2) Corporation Science Park, Taras Shevchenko University of Kyiv, Ukraine

3) Université Lyon 1, CNRS, Institut Lumière Matière, France

4) Institute of High Technologies, Taras Shevchenko National University of Kyiv, Ukraine

5) University of Lyon, CarMeN Laboratory, INSA de Lyon, France

\* skryshevsky AT knu.ua

Carbon dots (CDs) have attracted considerable attention as fluorescent nanomaterials for biomedical applications owing to their excellent biocompatibility, low toxicity, tunable photoluminescence, and simple synthesis routes compared to traditional semiconductor quantum dots [1-3]. In particular, red-emitting carbon dots are highly desirable for bioimaging because they offer deeper tissue penetration, reduced autofluorescence background, and lower phototoxicity. This study reports a novel one-pot hydrothermal synthesis of biocompatible red-emitting fluorinated carbon dots ( $R_5F$ ) using citric acid, urea, and m-trifluoromethylaniline as precursors in N,N-dimethylformamide medium. The obtained  $R_5F$  carbon dots were thoroughly characterized by dynamic light scattering (DLS), zeta-potential measurements, UV-Vis absorption spectroscopy, and fluorescence excitation-emission mapping. The particles exhibit a narrow size distribution in the range of 1-6 nm with a maximum at approximately 2 nm and demonstrate excellent colloidal stability in the physiological pH range, with zeta potential values below -20 mV at  $pH \geq 8$ . Optical studies revealed multiple absorption bands corresponding to  $\pi \rightarrow \pi^*$  and  $n \rightarrow \pi^*$  transitions, along with strong red photoluminescence efficiently excited in the broad visible range (420-520 nm). Cytotoxicity evaluation performed on 3T3-L<sub>1</sub> fibroblast cells using real-time xCELLigence RTCA system showed high biocompatibility at concentrations up to 0.3 mg/mL, with no significant impact on cell proliferation. Fluorescent microscopy confirmed effective cellular uptake and bright red labeling primarily localized in the cytoplasm without any visible alterations in cell morphology or viability. Taken together, these findings demonstrate that the synthesized fluorinated carbon dots possess outstanding optical properties and excellent biocompatibility, making them highly promising, non-toxic fluorescent probes for longterm cell imaging, biomedical diagnostics, and other theranostic applications.

**KEYWORDS:** Fluorinated carbon dots, Fluorescence, Bioimaging, Optical properties, Cytotoxicity

**ACKNOWLEDGEMENTS:** This work was financially supported by EU Horizon 2020 Research and Innovation Staff Exchange Programme (RISE) under Marie Skłodowska-Curie Action (project “UNAT” No.101008159), National Research Foundation of Ukraine (project 2025.07/0098) and by Ministry of Education and Science of Ukraine (project 26BF07-03).

### REFERENCES

- [1] M. Liu, “Optical Properties of Carbon Dots: A Review,” *Nanoarchitectonics*, 1, 1-12 (2020).
- [2] A. Topchylo, K. Paliienko, A. Zaderko, T. Nychporuk, A. Géloën, O. Pylypova, I. Ivanov, V. Skryshevsky, V. Lysenko, Gd<sup>3+</sup>-Doped Biocompatible Fluorinated Carbon Dots for Bimodal Bioimaging Applications, *ACS Applied Nano Materials*, 8, 19453-19463 (2025).

## Oxidase-like and peroxidase-like activities of CeO<sub>2-x</sub> nanoparticles stimulating quercetin oxidation at neutral and slightly acidic pH

V. Seminko<sup>1</sup>\*, N. Kavok<sup>1</sup>, G. Dudetskaya<sup>1</sup>, P. Maksimchuk<sup>1</sup>, V. Klochkov<sup>1</sup>

*1) Institute for Scintillation Materials, NAS of Ukraine, Ukraine*

\* seminko AT ukr.net

The potential anticancer effect of quercetin (3, 3', 4', 5, 7-pentahydroxyflavone) is related to ROS (reactive oxygen species) generation accompanying the processes of autoxidation of quercetin molecules [1]. At the same time, this approach suffers from the fact that autoxidation of quercetin occurs preferably at alkaline pH (~10), while the medium of cancer cells is slightly acidic (pH ~ 6.1-6.9). At these pH values the spontaneous oxidation rates of quercetin are too slow to produce ROS in concentrations sufficient to hamper the growth or metabolism of tumor cells.

The rate of quercetin autoxidation can be sufficiently increased by both external conditions (pH, temperature) and presence of catalysts. In this study, we demonstrate a significant enhancement of quercetin oxidation in the presence of CeO<sub>2-x</sub> nanoparticles observed not only at alkaline pH, but even at neutral and slightly acidic pH conditions (6.7-7.8). The experiments were carried out in the presence of O<sub>2</sub> and/or H<sub>2</sub>O<sub>2</sub> as oxidants. The effect of combination of H<sub>2</sub>O<sub>2</sub> and CeO<sub>2-x</sub> NPs on the quercetin oxidation rate strongly overcomes the influence of these two components alone confirming their synergistic action. The origin of this synergy can be related to catalytic (peroxidase-like) activity of CeO<sub>2-x</sub> NPs, i.e. the ability of these NPs to enhance the processes of oxidation of substrates (in this case, quercetin) by hydrogen peroxide. Kinetic analysis shows that the experimental data can be well described by the Michaelis-Menten model, confirming enzyme-like (oxidase- and peroxidase-mimicking) activities of CeO<sub>2-x</sub> NPs. The high catalytic activity of CeO<sub>2-x</sub> nanoparticles can be attributed to the favorable redox potential of the Ce<sup>3+</sup>/Ce<sup>4+</sup> couple, which facilitates efficient electron transfer and promotes quercetin oxidation under these conditions.

---

**KEYWORDS:** Quercetin, Nanoceria, Cancer, Reactive oxygen species

---

**ACKNOWLEDGEMENTS:** This research was supported by National Research Foundation of Ukraine, Grant № 2023.03/0050.

---

### REFERENCES

[1]

A. Rauf, M. Imran, I.A. Khan, M. ur-Rehman, S.A. Gilani, Z. Mehmood, M.S. Mubarak, Anticancer potential of quercetin: A comprehensive review

# Track 12

Enabling Technologies and Emerging Directions

## Exploiting the dynamical properties of nanoscale memristors for efficient information processing

A. Halbritter<sup>1</sup>\*

*1) Department of Physics, Institute of Physics, Budapest University of Technology and Economics, Hungary*

\* halbritter.andras AT ttk.bme.hu

Memristive devices are commonly benchmarked by the multi-level programmability of their resistance states. Neural networks utilizing memristor crossbar arrays as synaptic layers largely rely on this feature. However, these “static” applications leave the rich dynamical properties of memristors largely unexploited. These dynamic features include not only the availability of ultra-short switching times of 10ps [1,2], but also the exponential voltage dependence of the resistive switching speed and the tunability of the dynamic fluctuations by voltage manipulation [3]. In my talk, I will review how such dynamical features can be used for efficient information processing, such as (i) solving complex computational problems with memristive Hopfield neural networks [4], or (ii) performing time series analysis and prediction with dynamical memristor circuits [5].

---

**KEYWORDS:** Neuromorphic computing, Memristors, Reservoir computing, Time series prediction

---

**ACKNOWLEDGEMENTS:** The NKFI K143169 and 152611 research grants are acknowledged.

---

### REFERENCES

- [1] M. Csontos, Y. Horst, N.J. Olalla, U. Koch, I. Shorubalko, A. Halbritter, J. Leuthold, Picosecond Time-Scale Resistive Switching Monitored in Real-Time, *ADVANCED ELECTRONIC MATERIALS* 9, 2201104 (2023)
- [2] Schmid, Sebastian Werner ; Posa, Laszlo ; Torok, Tímea Nora ; Santa, Botond ; Pollner, Zsigmond ; Molnar, Gyorgy ; Horst, Yannik ; Volk, Janos ; Leuthold, Juerg ; Halbritter, Andras; Csontos, Miklós, Picosecond Femtojoule Resistive Switching in Nanoscale VO<sub>2</sub> Memristors, *ACS NANO* 18, 21966 (2024)
- [3] Nyáry, Anna ; Balogh, Zoltán ; Sánta, Botond ; Lázár, György ; Jimenez, Olalla Nadia ; Leuthold, Juerg ; Csontos, Miklós ; Halbritter, András, Benchmarking Stochasticity behind Reproducibility: Denoising Strategies in Ta<sub>2</sub>O<sub>5</sub> Memristors, *ACS APPLIED MATERIALS & INTERFACES* 17, 25654 (2025)
- [4] Fehérvári, János Gergő ; Balogh, Zoltán ; Török, Tímea Nóra ; Halbritter, András, Noise tailoring, noise annealing, and external perturbation injection strategies in memristive Hopfield neural networks, *APL MACHINE LEARNING* 2, 016107 (2024)
- [5] Molnár, Dániel ; Török, Tímea Nóra ; Volk, János ; Kövecs, Roland ; Pósa, László ; Balázs, Péter ; Molnár, György ; Olalla, Nadia Jimenez ; Balogh, Zoltán ; Volk, János, Leuthold, Juerg; Csontos, Miklós; Halbritter, András, Neural Information Processing and Time-Series Prediction with Only Two Dynamical Memristors, *ADVANCED ELECTRONIC MATERIALS* 12, e00353 (2026)

## Memristor-based physical reservoir computing for temporal signal classification at the edge

I. Tompris<sup>1</sup>, I. K. Chatzipaschalis<sup>1</sup>, T. P. Chatzinikolaou<sup>1</sup>, G. Kleitsiotis<sup>1</sup>, I. Fyrigos<sup>1</sup>, G. C. Sirakoulis<sup>1</sup>\*

1) Department of Electrical and Computer Engineering, Democritus University of Thrace, Greece

\* gsirak AT ee.duth.gr

Temporal signals are central to modern sensing, appearing in electroencephalogram (EEG) signals, electrocardiogram (ECG) recordings, and industrial vibration sensor metrics. Their classification remains difficult because such data are often noisy, nonstationary, artifact-contaminated, and governed by short- and long-range temporal dependencies [1]. Contemporary machine learning approaches can address these challenges, but they frequently require extensive preprocessing, recurrent architectures, or large training datasets, limiting their suitability for compact edge hardware [2]. Reservoir computing offers an alternative by projecting input sequences into a high-dimensional dynamical space, where temporal structure can be separated using a simple readout [3]. However, realizing such reservoirs in physical hardware remains challenging, particularly when nonlinear dynamics, fading memory, recurrent interaction, and sensor-compatible input encoding must be integrated within a compact substrate. In this work, a mycelium-inspired reservoir can successfully perform generalized temporal data classification by exploiting the echo state property of a memristive oscillator network. Herein, biological inspiration is drawn from mycelium’s electrical spiking behavior, which informs the nonlinear oscillatory response at the cell level, and from its small-world network topology, characterized by high local clustering and short global path lengths, defining the reservoir’s connectivity [4]. In this architecture, temporal samples are injected through an input layer and mapped onto a memristive oscillator grid composed of up to several hundred coupled oscillatory neurons. The resulting reservoir dynamics are then analyzed for each data sample through several physically interpretable features, including oscillation waveform amplitude, DC level, frequency, and RMS energy. These features form the extracted reservoir state and are passed to a single affine readout layer for classification. The combination of small-world topology and echo-state dynamics enables the reservoir to transform noisy temporal inputs into separable dynamical representations, which can be successfully classified by a readout layer. In addition, the generalized input interface makes the reservoir compatible with sensory front ends, including electrophysiological, optical, chemical, or mechanical sensing systems. These results position memristive oscillator reservoirs as promising hardware substrates for sensor-flexible temporal classification, with potential relevance to biomedical monitoring and low-power edge intelligence towards multi-modal sensing neuromorphic hardware.

---

**KEYWORDS:** Memristive oscillatory networks, Physical reservoir computing, Bio-Inspired neuromorphic computing, Temporal data classification, Mycelium-Inspired networks

---

**ACKNOWLEDGEMENTS:** This research work was supported by the FUNGATERIA project, which received funding from the European Union’s HORIZON-EIC-2021-PATHFINDER CHALLENGES program under grant agreement no. 101071145.

### REFERENCES

- [1] I. K. Chatzipaschalis, I. Tompris, P. Fraidakis, I.-A. Fyrigos, A. Rubio, and G. C. Sirakoulis, “Electroencephalogram-driven recognition of parkinson’s disease through a mycelium-inspired memristive reservoir computing circuit,” *Advanced Intelligent Systems*, p. e202501384, 2026.
- [2] T. P. Chatzinikolaou, A. Mavropopoulis, I. Tompris, G. Kleitsiotis, I. K. Chatzipaschalis, K.-A. Tsakalos, I.-A. Fyrigos, M.-A. Tsompanas, A. Adamatzky, P. Dimitrakis *et al.*, “Enabling mycelium-inspired reservoir computing with memristive oscillating cellular automata,” in *2025 IEEE International Symposium on Circuits and Systems (ISCAS)*. IEEE, 2025, pp. 1-5.
- [3] G. Zhang, J. Qin, Y. Zhang, G. Gong, Z.-Y. Xiong, X. Ma, Z. Lv, Y. Zhou, and S.-T. Han, “Functional materials for memristor-based reservoir computing: Dynamics and applications,” *Advanced Functional Materials*, vol. 33, no. 42, p. 2302929, 2023.
- [4] I. Tompris, I. K. Chatzipaschalis, T. P. Chatzinikolaou, G. Kleitsiotis, K.-A. Tsakalos, I.-A. Fyrigos, M.-A. Tsompanas, A. Adamatzky, P. Ayres, and G. C. Sirakoulis, “Mycelium as a computational medium: a framework for growth modeling towards reservoir computing: I. Tompriset al.” *Natural Computing*, vol. 24, no. 4, pp. 829-843, 2025.

## **Direct atomic layer processing (DALP®): Spatially localized, multi-material fabrication for next-generation devices from discovery to manufacturing**

M. Plakhotnyuk<sup>1\*</sup>, M. Baraket<sup>2</sup>

1) ATLANT 3D Nanosystems, Kongens Lyngby, Denmark

2) ATLANT 3D Nanosystems, Taastrup, Denmark, Denmark

\* mp AT atlant3d.com

Progress in next-generation advanced electronic and functional devices, based on complex heterostructures and advanced materials integration, is increasingly constrained by the rigidity of conventional thin-film processing and patterning workflows. While these approaches deliver high material quality and uniformity, they offer limited flexibility for spatially localized, multi-material fabrication, three-dimensional thickness engineering, and rapid experimentation at the nanoscale within a single process flow.

ATLANT 3D introduces Direct Atomic Layer Processing (DALP®), a nanofabrication technology enabling digitally controlled, spatially localized deposition of multiple materials with atomic-scale precision. DALP allows different materials to be deposited sequentially and locally in a unified workflow, enabling manufacturing of complex material stacks, heterostructures, interfaces, and thickness gradients without intermediate lithographic patterning steps.

This presentation describes the DALP process architecture and its role in both combinatorial materials discovery and targeted device manufacturing for next-generation devices. By enabling programmable material placement, controlled thickness variation, and repeatable execution within a single platform, DALP supports accelerated materials exploration while also enabling the direct production of device-ready structures as part of broader manufacturing flows. Representative examples include multi-material nanoscale structures for advanced semiconductor and functional material applications, where precise interface control, spatial selectivity, repeatability, and manufacturability are critical. DALP expands the accessible design space of nanoscale fabrication and provides a direct pathway from materials discovery to device-ready, manufacturable structures.

---

**KEYWORDS:** Nanofabrication, ALD, DALP, Atomic layer processing

## Understanding the structure to mechanics relationships in 3D printed nanoporous membranes

L. Carvalho<sup>1</sup>\*, H. Balakrishnan<sup>1</sup>, L. Dumée<sup>2</sup>, K. Askar<sup>3</sup>, H. Arafat<sup>4</sup>

1) Research & Innovation Center for Graphene and 2D Materials (RIC-2D), Khalifa University, Abu Dhabi, United Arab Emirates

2) Curtin University, Perth, Australia, Australia

3) Ministry of Higher Education & Scientific Research, Abu Dhabi, United Arab Emirates

4) Khalifa University, Abu Dhabi, UAE, United Arab Emirates

\* 100064526 AT ku.ac.ae

Here, we present a design-driven fabrication strategy that integrates digital light processing (DLP) 3D printing with an established overall chemistry used on the fabrication of porous monoliths for chromatography, known as polymerization-induced phase separation (PIPS), to enable the formation of nanostructured porous materials beyond the intrinsic resolution limits of additive manufacturing. In this approach, monomers and pore-forming agents are polymerized in situ during printing, driving phase separation at the nanoscale and generating high-density symmetric nanoporous networks with controlled pore cavity dimensions. This strategy decouples macroscopic architecture from nanoscale pore formation, allowing their independent control within a single manufacturing step.

However, there is still limited data availability and understanding of the mechanical behaviour of photopolymerized nanoporous structures and how the polymerization kinetics interfere in the densification and microcrack formation often seen in post-processing and pressurized operations such as membrane filtration. This is predominantly due to the fact that stress distribution is uneven, tending to concentrate in pore walls and thus making it highly dependent on internal pore distribution and structure density. Our 3D printed membranes have a symmetrical sponge-like pore structure with size distribution between 12 and 25 nm, with a mean pore of 19 nm and thickness printing ranging from 100 to 400  $\mu\text{m}$ . We aim to understand their compressive behaviour and the impact that integrating phase separation in situ during network development has on it by mimicking pressure-driven operations similar to those achieved during membrane filtration.

The main objective of our work is to embed the mechanical response of the 3DP membranes as a design parameter within the printing process, rather than treating mechanical compaction as an inevitable consequence of the fabrication process. The strategy combined controlled compression testing with cross-flow filtration experiments up to 6 bar to quantitatively link pressure-induced strain to changes in membrane porosity, pore size distribution and permeability. By correlating mechanical behavior with operational performance, we were able to monitor plastic compaction and creep behavior of the specimens, benchmarking it against commercial poly(amide) membranes which enables rational optimization of membrane fabrication for improved compaction resistance. Although demonstrated here in the context of membrane fabrication, this work establishes a new method to assess the mechanical stability and performance of nanoporous materials.

---

**KEYWORDS:** 3D printing, Polymerization induced phase separation (PIPS), Mechanical behavior, Membranes, Nanopores

---

**ACKNOWLEDGEMENTS:** This research was funded by Khalifa University of Science and Technology through the Court of Presidential Affairs program under Project ID: KU-EXT-8434000443-20238434000443 and supported by the Research & Innovation Center for Graphene and 2D Materials, Khalifa University of Science and Technology (KU-RIC2D).

---

### REFERENCES

- [1] H. Kalathil Balakrishnan, S. M. Lee, L. F. Dumée, E. H. Doeven, R. Alexander, D. Yuan, and R. M. Guijt, "3D printed integrated nanoporous membranes for electroextraction of DNA," *Nanoscale*, 15(24), 10371-10382 (2023).
- [2] H. K. Balakrishnan, L. F. Dumée, A. Merenda, C. Aubry, D. Yuan, E. H. Doeven, and R. M. Guijt, "3D Printing Functionally Graded Porous Materials for Simultaneous Fabrication of Dense and Porous Structures in Membrane-Integrated Fluidic Devices," *Small Structures*, 4(5) (2023).

Posters

T12-05

POSTER

**Analysis of low and high linear transfer radiation effects on data carrying DNA origami templates**

K. Cardos<sup>1\*</sup>, L. Sala<sup>1</sup>, J. Kočišek<sup>1</sup>

1) J. Heyrovský Institute of Physical Chemistry of the CAS, Czech Republic

\* karen.cardos AT jh-inst.cas.cz

DNA has become an alternative material for data storage because of its high information density, sustainability, stability, and longevity [1]. An interesting means of data storage represents patterns of objects placed on DNA Origami nanostructures (DON). The DON technique allows to build any desired shape by folding a plasmid single strand, known as scaffold, with complementary short single strands, called staples[2]. Another feature is the precise addressing of organic or inorganic molecules on the template by staple extensions [3]. However, it's necessary to prove the efficiency and durability of DONs for data storage. In this project, we used Keller's group DONs design and streptavidin protein in defined patterns to support digital information encoding, storage, and retrieval [4].

As a first step, we show how streptavidin interacts with the origami structure and how variations in concentration, deposition conditions, and substrates affect binding yield in a specific arrangement. Additionally, since long-term data storage is the target application, a key aspect is simulating cumulative degradation by exposing DONs to ionizing radiation, specifically low-LET 16 MeV electrons and high-LET 1.5 GeV <sup>16</sup>O<sup>8+</sup> projectiles [5]. This work focuses on the effects of radiation type, the presence of streptavidin during irradiation, binding configuration, and radical scavenger concentration on the sensitivity of the encoded patterns to radiation damage. The results provide proof of concept for scalable, efficient, and explored strategies for enhancing the long-term data preservation capabilities of nanostructures, contributing to the development of next-generation data storage technologies.

**KEYWORDS:** DNA origami, Data storage, Radiation

**ACKNOWLEDGEMENTS:** Acknowledgment: This work was supported by the European Union via project number 101115317, NEO (neodna.eu).

**REFERENCES**

- [1] A. Doricchi, C. M. Platnich, A. Gimpel, F. Horn, M. Earle, G. Lanzavecchia, A. L. Corajarena, L. M. Liz-Marzán, N. Liu, R. Heckel, R. N. Grass, R. Krahne, U. F. Keyser, and D. Garoli. "Emerging Approaches to DNA Data Storage: Challenges and Prospects". ACS Nano, 26, (2022).
- [2] P. W. Rothemund. "Folding DNA to create nanoscale shapes and patterns". Nature, 440, 297-302(2006).
- [3] N. V. Goigt, T. Tørring, A. Rotaru, M. F. Jacobsen, J. B. Ravnsbæk, R. Subramani, W. Mamdouh, J. Kjems, A. Mokhir, F. Besenbacher, and K. V. Gothelf. "Single-molecule chemical reactions on DNA origami". Nature Nanotechnology, 5, 200-203(2010).
- [4] L. Rabbe, E. Tomm, G. Grundmeier and A. Keller. "Toward high-density streptavidin arrays on DNA origami nanostructures". RSC Advances, 30, (2026).
- [5] J. Ameixa, L. Sala, J. Kocišek, I. Bald. "Radiation and DNA Origami Nanotechnology: Probing Structural Integrity at the Nanoscale". ChemPhysChem, 26(1), 1-17(2024).

## Next-generation flexible pem fuel cells enabled by MXene nanomaterials

A. Marinoiu<sup>1\*</sup>, M. Varlam<sup>2</sup>

1) Institute for Cryogenics and Isotopic Technologies - ICSI, Ramnicu Valcea, Romania, Romania

2) Institute for Cryogenics and Isotopic Technologies - ICSI, Rm Valcea, Romania

\* adriana.marinoiu AT icsi.ro

The vision of our work is to develop a lightweight, flexible, and high-performance PEM fuel cell platform by integrating MXene-based nanomaterials to enhance conductivity, durability, and water management-targeting emerging applications in wearables, UAVs, and portable power systems. The ongoing project will develop a new generation of flexible proton exchange membrane (PEM) fuel cells by integrating MXene nanomaterials into key components of the system. MXenes, a class of highly conductive and hydrophilic 2D materials, offer significant advantages in improving electrical conductivity, catalyst efficiency, and water management, while also enabling mechanical flexibility. By incorporating MXenes into the catalyst layer, membrane, and gas diffusion layer, the project seeks to enhance overall fuel cell performance, reduce reliance on precious metals such as platinum, and improve durability under dynamic operating conditions.

The core Innovation part is to integrate MXene type materials into key PEMFC component -a) Catalyst Layer Enhancement -MXene-supported catalysts (Pt/MXene or non-PGM) in order to improve catalyst dispersion, electron transport and reduce Pt loading and b) Gas Diffusion Layer (GDL) Engineering MXene coating for optimization of water transport and enhance durability under flex conditions.

Basic work are now to solve main technical challenges related to MXene oxidation and long-term stability, scalable and reproducible MXene synthesis and Mechanical durability under repeated flexing

The resulting technology will deliver lightweight, bendable, and high-performance fuel cells suitable for emerging applications such as UAVs, wearable devices, and portable power systems. In addition to targeting higher power density and improved efficiency, the project addresses key challenges related to material stability, scalability, and integration into flexible architectures. Ultimately, this initiative positions itself at the intersection of hydrogen energy and advanced nanomaterials, contributing to the development of next-generation, adaptable energy solutions and strengthening capabilities in deep-tech innovation.

---

**KEYWORDS:** Lightweight, Flexible PEM fuel cell, MXenes, Portable power systems

---

**ACKNOWLEDGEMENTS:** National Authority for Scientific Research (Romania) (ANCS) provided financial support for this work through the projects PN 23 15 01 03, Contract no. 20N/2023 and by the project RO-HydroHub “Romanian Hydrogen and New Energy Technologies Hub”, contract nr. G2025-113330/ 2025, SMIS code: 351358, financed from European funds via the POCIDIF 2021-2027 Program.

## Luminescent silver-MOF platform for highly sensitive detection of glutathione

J. M. George<sup>1</sup>\*, G. Mohanta<sup>1</sup>, A. Sharma<sup>2</sup>

1) *AcSIR, CSIR-CSIO, Chandigarh, India*

2) *Amity School of Chemical Sciences, Amity University Punjab, India*

\* jiyagk317 AT gmail.com

Glutathione (GSH) is a crucial metabolite and antioxidant that is markedly elevated in the microenvironment of tumour tissues relative to normal tissues, making it an valuable biomarker for cancer diagnosis and therapy monitoring. For clinical diagnostics and biological research, accurate and timely detection of GSH is very vital. Recently, silver (Ag)-based metal organic frameworks (MOFs) have gained significant research interest due to their potential application in sensing and detection, bioimaging, and light-emitting devices. Herein, we report the synthesis and sensing performance of highly luminescent silver-based MOF derived from benzenedicarboxylic acid (BDC) as organic linker. Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), Thermogravimetric analysis (TGA), X-ray photoelectron spectroscopy (XPS) was used to confirm the successful synthesis. Harnessing the strong fluorescence of synthesized Ag-MOF and chemical affinity of constituent silver ions with thiol (-SH) groups, we demonstrate highly sensitive detection of glutathione molecules in simulated buffer solutions. The fluorescence quenching mechanism and the optimization of experimental parameters that maximize the quenching efficiency was also evaluated. Finally, the suggested assay was validated using spiked bovine serum samples, showcasing its practical implementation in biomedical research.

---

**KEYWORDS:** AgMOF, GSH, Fluorescent probes, TME

---

**ACKNOWLEDGEMENTS:** The authors gratefully acknowledge the support provided by their host institution for laboratory facilities and instrumentation. We sincerely thank the central instrumentation facility for access to FTIR, XRD, TGA, and XPS characterization tools.

---

### REFERENCES

- [1] Meister, A. Alton; Anderson, Michael E. Glutathione. *Annual Review of Biochemistry*, 1983, 52, 711-760.
- [2] Traverso, Nicola *et al.* Role of glutathione in cancer progression and chemoresistance. *Oxidative Medicine and Cellular Longevity*, 2013.
- [3] Feng, Dawei; Zhou, Hong-Cai Metal-organic frameworks for biomedical applications. *Chemical Society Reviews*, 2017, 46, 570-590.
- [4] Kreno, Lauren E. *et al.* Metal-organic framework materials as chemical sensors. *Chemical Reviews*, 2012, 112, 1105-1125.

## Biomedical nanotechnology in Ukraine: Biosafety and policy aspects

N. Inshyna<sup>1, 2 \*</sup>, I. Chorna<sup>3</sup>

1) Sumy State University, Sumy, Ukraine

2) Sumy National Agrarian University, Ukraine

3) Biomedical Research Center, Academic and Research Medical Institute, Sumy State University, Sumy, Ukraine

\* n.inshina AT med.sumdu.edu.ua

The rapid development of modern biomedical nanotechnologies underscores the need to develop new approaches to regulate biosafety issues, as well as the legal and social aspects of this field. In the context of the sustainable development strategy, this area is becoming not merely a subject of scientific interest but the foundation of a new bioeconomy. The aim of this study is to assess and clarify the specific features of the legislative regulation of research in this field at the national level.

To achieve the study's goal, an analysis of key Ukrainian normative documents available on the relevant official website (<https://zakon.rada.gov.ua>) was conducted to determine whether the legislation specifically contains the terms “nanotechnology”, “nanomaterial”, “nanoparticle”, “nanomedicine”, “nanorobot”, etc.

The review of selected open-source normative documents indicates that terms with the prefix “nano” are not explicitly mentioned in these texts. Instead, these documents establish the broader biomedical and biosafety context into which nanomedicine is implicitly integrated, highlighting a distinct gap in nano-specific regulatory policies. The priority areas for the development of nanobiotechnologies in Ukraine include the creation of biomaterials for regenerative medicine, the development of biosensors, the biofunctionalisation of nanomaterials, the development of innovative technologies for controlled drug delivery, and biomedical imaging. Despite the enormous prospects, the use of nanomaterials requires strict biosafety control - strategic risk management for human life and environmental conditions.

In Ukraine, the legal regulation of biomedical nanotechnologies is currently undergoing active transformation and integration into the European Union (EU) acquis. At the legislative level, the regulation of legal aspects in this field is distributed across laws on healthcare and innovation. Within the framework of the Association Agreement with the EU, Ukraine has undertaken the obligation to harmonise its national legislation with European norms. This concerns several critical dimensions: 1. intellectual property: the development of “purple biotechnology” (patenting) is a mandatory condition for attracting investment; 2. regulation of novel food products: according to Regulation (EU) 2015/2283 of the European Parliament and of the Council, any innovative food or medical products created using nanomaterials must undergo a rigorous risk assessment procedure before entering the market; 3. institutional transparency: the effective functioning of the sector is possible only on the condition of overcoming corruption and creating an independent judicial system that guarantees the rule of law for developers and consumers.

---

**KEYWORDS:** Nanobiotechnology, Nanomedicine, Bioengineering, Biosafety, Legislative regulation

---

**ACKNOWLEDGEMENTS:** Supported by project #0126U000874 of the Ministry of Education and Science of Ukraine.

## Scientometric analysis of research papers on artificial intelligence in nano-optics

I. Balagura<sup>1</sup>, I. Gorbov<sup>1</sup>\*, A. Kryuchyn<sup>2</sup>

1) University of Nottingham, United Kingdom

2) Institute for Information Recording, NAS of Ukraine, Ukraine

\* ivan.gorbov AT nottingham.ac.uk

AI research methods such as natural language processing, image recognition, machine learning, and others are widely applied in most research fields, enabling automation, big data analysis, pattern recognition, and intelligent decision-making [1]. Machine learning (ML), a core branch of artificial intelligence, has recently emerged as a transformative tool in nano-optics, enabling new approaches for faster simulations, efficient inverse design, and automated optimization of complex nanophotonic systems [2,3]. By examining the intersection of AI and nano-optics, this work seeks to contribute to a deeper understanding of current developments, research gaps, and future directions in this rapidly evolving field.

Here we show a scientometric analysis of AI and machine learning applications in nano-optics, utilizing data from 57,924 papers in the Scopus database. The research aims to examine the role of AI, quantify its presence in nano-optics, and assess its impact using subject-domain mapping and complex networks. The study highlights significant growth in publications since 2021 from 4,186 papers in 2021 to 13,419 papers in 2025, identifying four major research clusters that bridge computational methods, such as "deep learning", with physical applications like "metasurface" and "surface plasmon resonance". Through network mapping, we have pinpointed the most influential journals and author collaborations that are currently dictating the field's trajectory. These findings indicate that the field is shifting away from theoretical modeling toward practical, AI-enhanced performance metrics in materials like "perovskite".

Our results demonstrate the dynamic changes in keywords by years, revealing trends in AI and nano-optics. Among the most common keywords in 2025 and 2026 are "inverse design", "SERS", "surface plasmon resonance", "metasurface", and "graphene". As computational methods and data availability continue to improve, ML is expected to play an increasingly central role in advancing both fundamental research and practical applications in nano-optics. Machine learning is transforming nano-optics from a simulation-driven field into a data-driven, design-optimized discipline, enabling faster discovery, smarter devices, and entirely new optical functionalities.

---

**KEYWORDS:** Scientometrics, Artificial intelligence, Machine learning, Nano-optics, Co-word networks

---

**ACKNOWLEDGEMENTS:** Iryna Balagura and Ivan Gorbov acknowledge support from the British Academy and the University of Nottingham through the Researchers at Risk Fellowships Programme (RaR\100215, RaR\100182).

---

### REFERENCES

- [1] S. Yuan, Z. Shao, X. Wei *et al.*, "Science behind AI: the evolution of trend, mobility, and collaboration", *Scientometrics*, 124, 993-1013 (2020).
- [2] R. Peter. Wiecha, Arnaud Arbouet, Christian Girard, and Otto L. Muskens, "Deep learning in nano-photonics: inverse design and beyond", *Photonics Research*, 9(5), B182-B200 (2021).
- [3] J. J. Mim, A. A. Mamun, M. H. Nayem, S. Mahmud, A. Nath, SM Maksudur Rahman, Shekh Asraful Fidal, Nayem Hossain, "Machine learning-driven advances in nanotechnology: From materials design to process optimization - A review", *Materials Today Communications*, 50 114485 (2026).

## Author Index

---

- Abbas, S. A. 75  
Abouelela, M. 199  
Achinuq, B. 151  
Adamiak, S. 119  
Adamiv, V. 45  
Adelung, R. 210  
Afonso, Y. F. 217  
Aguiar, I. 239  
Ahmed, E. M. S. 275  
Akbar, Z. 28  
Akben, H. K. 241  
Akkuş, S. 57  
Akopova, O. 276  
Aksimentyeva, O. 229  
Aksoy, B. T. 70  
Akutagawa, T. 110, 125  
Alejandro, J. M. 245  
Alex, S. G. 167  
Ali, S. 68  
Aljedani, J. 63  
Alonso, J. A. 12  
Alotibi, S. 244  
Amato, M. 14  
Ameloot, R. 210  
Ameri, T. 210  
Anasori, B. 6  
Andrushchak, A. 45  
Andrushchak, H. 226  
Andzane, J. 255, 93  
Angelova, L. 123  
Anwar, N. 28  
Anwar, S. H. 28  
Arafat, H. 295  
Arce, D. D. R. 209  
Arif, M. 28  
Ashatov, A. 134  
Askar, K. 295  
Assaf, B. A. 195, 172  
Azizi, S. 28  
Babar, Z. 74  
Bagday, S. 148  
Baginskyi, I. 77  
Bajkacz, S. 50  
Bakalo, A. 281  
Balagura, I. 300  
Balakrishnan, H. 295  
Balciunaite, A. 184  
Banach, M. 26  
Baraban, L. 271  
Baraket, M. 294  
Barcellos, T. 245  
Barlas, T. 242  
Barman, A. 181  
Barthaburu, M. E. P. 239  
Barylyak, A. 140  
Baránek, M. 203  
Basnukaeva, R. 41, 139  
Batjuka, A. 260  
Baumgarten, J. 198  
Bazaliy, Y. 170  
Bechelany, M. 216  
Belous, A. 173, 177  
Bendak, A. 45  
Bendinskaite, S. 212  
Benešová, M. 209  
Beni, V. 217  
Beresnev, V. 120  
Berezina, A. 46  
Berezovska, N. 254, 242  
Berger, A. 156  
Bertran-Llorens, S. 217  
Bezsmertna, O. 161  
Bhalla, V. 273, 287  
Bhardwaj, P. 48  
Bharti, B. 287  
Bi, H. 85  
Bielska, B. 282  
Bilgen, E. 19  
Bilous, A. 279  
Bisht, B. 273  
Bobitski, Y. 140  
Bodnarova, R. 90  
Bogatyrenko, S. 36  
Boguzaitė, R. 212  
Bojarski, P. 64  
Bokes, P. 180  
Bolatov, S. 137  
Bondar, Y. 247  
Borkovska, L. 147, 172  
Bozhko, N. 60  
Brasiunas, B. 208  
Braun, N. 104  
Brazys, E. 212  
Brincoveanu, O. 53  
Brinza, M. 210  
Brodnikovskiy, Y. 147  
Bsaibess, E. 20  
Bucher, G. 280  
Bui, T. T. A. 13  
Buitkenov, D. 130, 117  
Bulyha, I. 50, 61  
Bunyaev, S. 161  
Buravtseva, L. 41  
Buryanov, O. 286  
Byelinska, I. 268  
Běloušek, M. 111  
Cabal, B. 55, 65  
Cabaleiro, D. 243  
Cambel, V. 180  
Can, V. 19, 223  
Car, T. 123  
Cardos, K. 296, 209  
Caro, E. S. 245  
Carroll, D. 81  
Carvalho, L. 295  
Carvalho, S. 240  
Casoli, L. 222  
Castro, J. D. 240  
Cavaleiro, A. 240  
Cavaleiro, D. 240  
Caçador, A. 142  
Cegielka, D. 127, 113  
Chakraborti, S. 183  
Chalyy, D. 59  
Chamon, C. 85  
Charczuk, N. 274  
Chatzinikolaou, T. P. 293  
Chatzipaschalis, I. K. 293  
Chaudhary, V. 23  
Chauhan, A. 18  
Chaves, D. 199  
Chekailo, M. 119  
Cherednichenko, S. 41  
Chidambaram, R. J. 143  
Chiodi, F. 14  
Chmilenko, V. 249  
Chorna, I. 77, 299  
Chouhan, H. 143  
Chudinovych, O. 29  
Chukova, O. 147  
Chumak, A. 163  
Chumak, H. 177  
Cieniek, B. 119  
Cirik, V. 138  
Cools, I. P. 198, 199  
Coy, E. 15, 235  
Cremer, S. 104  
Cundrle, J. 261, 262  
Cyganiak, P. 127, 113, 114, 115  
Czerwiński, A. 101, 102  
Danylchenko, P. 220  
Danyliak, M. 126  
Daoud, L. 218  
Dargie, Z. A. 257  
Das, A. 7  
Daskalova, A. 123  
Dausy, H. 199  
Deineka, V. 135  
Dekura, S. 125  
Della Ventura, B. 74  
Demchenko, O. 286  
Demchenko, V. 129, 286, 131, 132  
Derecha, D. 186  
Devi, P. 76  
Ding, H. 80  
Disha, D. 37  
Dmytruk, A. 54  
Dmytruk, I. 254, 242  
Dmytruk, S. 50, 61  
Dobročka, E. 143  
Dolbin, A. 41  
Dolic, S. 234  
Dong, Z. 33, 34  
Drabavicius, A. 184  
Dubovsky, M. 261, 262, 248  
Dudetskaya, G. 278, 290, 232, 288  
Dudin, S. 36  
Dukhnovskiy, S. 77  
Dumanli, S. 19  
Dumée, L. 295  
Dvornichenko, A. 39, 40, 42, 128  
Dziedzic, A. 119  
Dziubenko, N. 268, 289

- Díaz-Ufano, C. 217  
Džerovski, S. 91  
Egyenes, F. 143  
El Hadri, H. 280  
El Kadib, A. 282  
Elitaş, M. 241  
Eliçatal, F. D. 176  
Elmers, H. 172  
ElRifai, J. 20  
Ercerg, I. 123  
Erdody, S. 221  
Erts, D. 255, 93  
Evans, R. F. L. 151  
Fantych, I. 192  
Fatima, M. 74  
Fedchenko, O. 172  
Fedorchuk, O. P. 177  
Fedotov, O. 224, 218  
Feilhauer, J. 174  
Fekete, L. 138  
Feldman, Y. 12  
Felinskyi, G. 146  
Felinskyi, S. 146  
Felsharuk, A. 255  
Fernández, A. 55, 65  
Filipovic, L. 13  
Finşgar, M. 91  
Folkestad, M. F. 22  
Frutos, M. M. 239  
Fukushima, T. 113  
Furdyna, J. 195, 172  
Fyrigos, I. 293  
G, D. K. 116  
Gaberšček, M. 91  
Gajovic, A. 234  
Galstian, I. 259  
Gamernyk, R. 148  
Garrido, F. 142, 144  
Gavars, D. 255  
Gavrila, R. 53  
Geloan, A. 289  
George, J. M. 298  
Gheorghe, A. 220  
Ghosh, S. 12  
Glavin, A. 283  
Gmitra, M. 200  
Gnatenko, K. 86  
Gogotsi, O. 208, 68, 77  
Golovynska, I. 224  
Golovynskyi, S. 224  
González-Fernández, S. 65  
Gorbov, I. 300, 221  
Gorbyk, P. 34  
Gouder, T. 167  
Gourbilleau, F. 118, 147  
Goyal, I. 76  
Grabowski, M. 142  
Grabowski, O. 101  
Graczyk, P. 181  
Grajcar, M. 203  
Grebnevs, V. 135  
Green, D. 85  
Gregušová, D. 143  
Grochowska, K. 15, 71  
Gromyko, O. 148  
Grygiel, M. 102  
Grygorova, G. 284, 285, 231  
Grygoruk, V. 146  
Grzanka, E. 142, 144  
Gucmann, F. 143  
Guichaoua, D. 45  
Gumieniak, J. 15, 71  
Gunjesh, A. 18  
Guziewicz, E. 144  
Güneş, B. 241  
Hadzaman, I. 58  
Halbritter, A. 292  
Hamankiewicz, B. 102  
Hamaya, K. 151  
Haniš, J. 200  
Hanuš, J. 106  
Harašta, S. 220  
Harmansah, C. 178  
Hassanien, A. 84, 194  
Hatashita, M. 105  
Havela, L. 167  
He, F. 221  
Heitmann, J. 118  
Heller, R. 144  
Henyh, J. 261, 262, 248, 263  
Hermida-Merino, C. 243  
Higginbotham, A. 85  
Hirohata, A. 171  
Hla, S. W. 82  
Hlek, Y. 265  
Horak, L. 167  
Horbenko, Y. 229  
Horský, M. 227  
Hozhdzinskyi, S. 33  
Hreb, V. 35  
Hrebelna, Y. 33  
Hrebynakha, V. 186  
Hrubišák, F. 143  
Hu, J. 21  
Hu, Y. 21  
Huber, F. 167  
Hubetska, T. 55, 65  
Hudec, B. 227  
Hunbin, O. 43  
Husak, Y. 50, 135, 61  
Huš, M. 91  
Hušeková, K. 143  
Hviščová, P. 128  
Iannotti, V. 74  
Iatsunskyi, I. 208  
Ichiyanagi, Y. 270, 172  
Ihnatenko, O. 33  
Ilashchuk, M. 226  
Inshyna, N. 299  
Iordache, M. 98  
Isler, A. 223  
Itakura, M. 155  
Ito, T. 277  
Iurzhenko, M. 131  
Ivan, K. 59  
Ivanenko, K. 33, 34  
Ivanov, O. 284  
Ivanov, V. 144  
Ivchenko, D. 265  
Jagadeesan, D. 76  
Jagerová, A. 111  
Jonáš, A. 209  
Jr, N. S. L. 138  
Junior, P. E. D. F. 200  
Juraev, N. 97  
Jureczko, P. 200  
Jóźwik, P. A. 142, 144  
Jędrzejewski, K. 100, 97  
Kabyletsykyi, D. 185  
Kadowaki, K. 179  
Kakazei, G. 161  
Kakimzhanov, D. 124  
Kalanov, D. 104  
Kalita, D. 144  
Kalmykova, T. 180  
Kalsoom, T. 72  
Kamataki, K. 105  
Kamimura, Y. 277  
Kara, E. 228, 188  
Karczewski, J. 15, 71  
Karlash, A. 54  
Karlicky, F. 72, 73  
Kartel, M. 33  
Karthikeyan, G. T. 248  
Kashiwagi, T. 179  
Kataoka, N. 270  
Kavok, N. 290, 232, 288  
Kawashima, H. 250  
Kaynts, D. 204  
Kazakova, O. 259  
Kenesbekov, A. 134  
Kennedy, T. 75  
Kentsch, U. 144  
Kepaptsoglou, D. M. 151  
Kera, S. 108  
Kern, S. 203  
Kerrigan, A. 151  
Keshtar, J. 143  
Khainakova, O. 55  
Khalak, V. 265  
Khan, S. I. 15  
Kharchenko, D. 39, 40, 62  
Kharchenko, V. 39, 40, 42, 128, 62  
Khliyeva, O. 265  
Khokhar, G. S. 22, 24  
Khokhlov, M. 38  
Khokhlova, J. 38  
Khomenko, A. V. 122  
Khomenkov, D. 118  
Khomenkov, V. 147  
Khomenkova, L. 147, 172  
Khort, P. 224, 218  
Khunou, B. P. 237  
Khursenko, S. 121  
Kienle, L. 104  
Kim, K. 94  
Kim, S. 109, 17  
Kim, Y. 243  
Kirakci, K. 262, 248  
Kisala, J. 140  
Klarák, J. 227  
Kleitsiotis, G. 293

- Klepko, V. 276  
Klochkov, V. 278, 290, 284, 231, 288  
Klym, H. 56, 58, 59  
Kobayashi, A. 155  
Kobylynska, N. 55, 65  
Koike, K. 155  
Koizumi, H. 171  
Kojic, V. 234  
Kolbjonoks, V. 258, 260  
Kolesnichenko, V. 29  
Kolos, M. 72  
Koloslkova, O. 167  
Komanicky, V. 185, 90  
Kondrakhova, D. 128  
Kondratenko, O. 195, 172  
Kordan, V. 229  
Korenkov, O. 60  
Korichev, S. 29, 30  
Kormunda, M. 111  
Korneichuk, A. 204  
Korniienko, V. 50, 61  
Korniy, S. 126  
Korposh, S. 221  
Korsunska, N. 147  
Kostin, V. 38  
Kostiv, O. 148  
Kostiv, Y. 56  
Kot, Y. 278, 232  
Kotko, A. 46  
Kotrusz, P. 13  
Kouao, D. 71  
Kousal, J. 25  
Koval, M. 226  
Kovalchuk, I. 253  
Kovchun, A. 281  
Kozak, A. 143  
Kozak, I. 186, 143  
Kozziarskyi, D. 225, 226  
Kozziarskyi, I. 225, 226  
Kozieł, K. 114  
Kozlica, D. 91  
Kozoriz, K. 147  
Kočišek, J. 269, 296, 209  
Kočišová, A. 106  
Krajewski, M. 101, 102  
Krakovský, I. 25  
Kramek, A. 15, 71  
Krasovska, M. 258  
Kravchenko, V. 121  
Krawczyk, M. 181  
Krettová, M. 143  
Krishnappa, M. 12  
Krtouš, Z. 25  
Krupka, O. 224, 218  
Krylov, S. 180  
Kryuchyn, A. 300  
Kucinskis, G. 93  
Kudelko, K. 249  
Kukhar, V. 177  
Kukurudziak, M. 225  
Kulesza, P. 97  
Kulibaba, V. 50, 61  
Kulyk, T. 186  
Kumar, B. M. 181  
Kumeda, M. 60  
Kuntyi, O. 35  
Kurpas, M. 13, 200  
Kurylov, B. 44  
Kusumoto, Y. 270  
Kutsevol, N. 31  
Kuzenko, S. 247  
Kuzenko, Y. 281  
Kuznietsova, H. 268, 289  
Kułak, L. 64  
Kvasnytskyi, B. 265  
Kvetková, L. 128  
Kyliań, O. 106  
Kyrylenko, S. 50, 77, 61  
Křivka, I. 25  
Laikhtman, A. 234  
Lamprecht, D. 13  
Lang, J. 45  
Lapchuk, A. 221  
Lari, L. 151  
Laurenčíková, A. 143  
Lavrynenko, O. M. 30  
Lazarov, V. K. 151  
Lebica, M. 127  
Lee, A. Y. 171  
Lee, H. 109, 17  
Leha, O. O. 149  
Lehninger, D. 118  
Leimane, I. L. 93  
Lejeune, N. 198  
Lemiesz, F. 102  
Len, E. 264, 259  
Leshchov, A. 252  
Levchenko, K. 162  
Li, L. 151  
Liedke, M. O. 144  
Lipińska, W. 15  
Lisova, O. 34  
Lisovskiy, V. 36  
Litra, D. 210  
Liu, X. 195, 172  
Liustrovaite, V. 208, 212  
Liutyi, A. 77, 61  
Livneh, T. 12  
Loboda, P. 52  
Loboda, V. B. 44, 121  
Lofaj, F. 128  
Lorenz, K. 142  
Lotnyk, A. 104  
Louis, S. 214  
Lugo, L. 243  
Lugovskoy, S. 257  
Lupan, C. 210  
Lupan, M. 284, 285, 231  
Lupan, O. 210  
Luzinov, I. 107  
Lyakhno, V. Y. 149  
Lysenko, I. 268, 289  
Lysenko, V. 268, 289  
Lytovchenko, S. 120  
Lytvynenko, Y. 172  
Maciej, A. 135  
Madsen, J. 13  
Magari, N. 210  
Mahalingam, V. 95  
Mahmoud, A. G. 75  
Maistruk, E. 225, 226  
Majetich, S. 151, 166  
Majkić, M. 11  
Makarov, D. 161  
Makhno, S. 33, 34  
Makhnyuk, I. 281  
Maksakova, O. 120, 204  
Maksimchuk, P. 278, 290, 284, 285, 231, 232  
Malanych, G. 251  
Malyshev, O. V. 193  
Malyshev, V. Y. 193  
Mamunya, Y. 47  
Mamykin, S. 254, 242, 195, 172  
Mano, Y. 155  
Manoryk, P. 254, 242  
Marinoiu, A. 256, 51, 98, 297  
Martinez, J. I. 12  
Martins, M. 91  
Martins, P. 91  
Maruzhenko, O. 47  
Marynin, A. 131, 132  
Marzegalli, A. 14  
Mason, N. 85  
Matsko, E. 35  
Matsueda, H. 83  
Matsuo, M. 171  
Matsushita, Y. 179  
Matulewicz, J. 142, 144  
Matyjasik, W. 26  
Maulit, A. 133  
Mazeika, K. 184  
Medvids, A. 79  
Meija, R. 93  
Melkov, G. A. 193  
Melnichuk, L. 118, 147  
Melnichuk, O. 118, 147  
Mereib, D. 20  
Meyer, J. C. 13  
Midlik, Š. 220  
Mieszczyński, C. 142, 144  
Mikalauskaite, A. 184  
Mikhailenko, V. 279, 283  
Minko, S. 267  
Mirković, J. 194  
Mishra, V. 95  
Misiura, A. 47  
Miłowska, K. 282  
Mlinarić, N. M. 272  
Mochalin, V. N. 69  
Mochiku, T. 179  
Moedl, E. 171  
Mohanta, G. 298  
Mohsenzadeh, E. 212  
Mohsin, S. 275  
Moitra, A. 18  
Molebnyi, O. 46  
Monastyrska, T. 46  
Morales, A. 213  
Morales, M. D. P. 217  
Mosbah, A. 189  
Muchiri, P. 14  
Muhammad, A. 75

- Mulenko, S. 264  
Muller, R. 53  
Mustonen, K. 13  
Mykhailova, H. 264  
Mykitovich, M. Z. 30  
Nabioldina, A. 130  
Nagpal, R. 210  
Nainggolan, B. 236  
Nakano, M. 155, 158  
Nakonechny, F. 257  
Nakonechnyi, S. 52  
Namvari, M. 67  
Nascimento, J. A. D. 151  
Nath, A. 246  
Navitski, I. 68  
Nawshad, M. 275  
Nebola, I. 204  
Nedelkoski, Z. 151  
Negishi, Y. 8  
Neilinger, P. 203  
Nekovei, R. 230  
Nemec, P. 227  
Nemeckova, Z. 261  
Nesterova, I. 93  
Neuhodov, Y. 232  
Nevmerzhytskyi, V. 32  
Nicolae-Maranciuc, A. 280  
Niemiec, M. 114  
Nikitchenko, Y. 288  
Nikitin, D. 25  
Nikolaienko, A. 54  
Nishino, F. 108  
Nogala, W. 37  
Nomngongo, P. N. 237  
Noto, L. L. 182  
Novotny, M. 73  
Nqayi, S. 182  
Nulens, L. 198, 199  
Nyaba, L. 237  
Nádaždy, P. 143  
Okamoto, S. 159  
Okubo, S. 155  
Oliseveca, I. 93  
Olszowska, K. 47  
Onat, Z. 178  
Onishchenko, A. 284, 231, 232  
Onodera, N. 125  
Orletskyi, I. 226  
Oue, D. 171  
Ozdil, Z. C. C. 19, 223  
Ozturk, Y. 176, 228, 57, 188, 178  
Pachauri, N. 95  
Pakstas, V. 184  
Palau, A. 202  
Palchik, A. 249  
Paliienko, K. 268  
Palys, B. 99, 100, 97  
Panda, D. 219  
Pankrác, J. 269  
Paraschenko, I. 47  
Parvulescu, C. 53  
Patrnčiak, M. 211  
Paulikaite, G. 184, 68  
Pavlović, M. 106  
Paziuk, L. 279  
Pazukha, I. 185, 43, 44, 136  
Perecko, T. 269  
Perčinić, M. 91  
Petjukevičius, A. 258, 260  
Pilipenco-Šleichertová, A. 138  
Pinchuk, A. 145, 254, 242  
Pintilie, S. 256  
Pirker, L. 209  
Pivko, P. 106  
Piñeiro, M. M. 243  
Plakhotnyuk, M. 294  
Plausinaitis, D. 215  
Pleceňik, T. 186, 211  
Plutenko, T. O. 177  
Podhurska, V. 98  
Pogorielov, M. 77, 61  
Pogrebnyak, A. 139  
Pohorelec, O. 143  
Ponomarova 249, 281  
Ponti, J. 280  
Poplauskas, R. 93  
Popov, A. 208, 68  
Popov, M. 173, 177  
Portier, X. 147  
Postolnyi, B. 139  
Potapenko, H. 34  
Precner, M. 203, 180  
Predanocny, M. 227  
Prentice, U. 215  
Pressé, S. 236  
Prinindya, K. N. N. 275  
Procházka, M. 106  
Prodanov, M. 122  
Prokopenko, O. V. 175, 187, 191, 192, 193, 196  
Prokopenko, V. 191  
Protiva, V. 209  
Prucnal, S. 144  
Pudiš, D. 143  
Pupel, K. 99, 97  
Puzrin, O. 38  
Pylypenko, O. 185, 43, 44, 136  
Pylypova, O. 268, 289  
Pylypovskiy, O. V. 161  
Piš, I. 203, 180  
R, J. 246  
Raes, B. 199  
Raghav, N. K. S. 22, 24  
Ragulya, A. 30  
Raisov, N. 117  
Rajh, T. 7  
Rakhadilov, B. 124, 133  
Ramanaviciene, A. 208, 68, 212  
Ramanavicius, A. 208  
Ramanavičius, A. 68, 212, 215  
Ramanavičius, S. 184, 68  
Ramasse, Q. 151  
Ramazashvili, R. 170  
Rana, B. 181  
Rao, K. P. 219  
Ratajczak, R. 142, 144  
Ratautaite, V. 212  
Rauf, M. 28  
Raveendran, A. 184, 68  
Redko, R. 254, 242  
Reniers, S. 199  
Rezunencko, S. 36  
Roberts, S. 236  
Roblegg, E. 272  
Roch, T. 211  
Roddatis, V. 104  
Rojek, A. 113  
Romanovska, N. 254, 242  
Romanyuk, O. 138  
Romanyuk, V. 242, 195, 172  
Ronduda, H. 102  
Roslyk, I. 77  
Rosová, A. 143  
Roy, A. 95  
Rozghon, Y. 42, 128  
Rozhdesvenska, L. 249  
Rud, M. 264  
Rudolph, M. 104  
Ruginyte, G. 212  
Rushkovsky, S. 286  
Rustemov, A. 133  
Ruta, S. I. 165, 190  
Rybalchenko, N. 286, 132  
Rymar, T. 252  
Rysanek, P. 261, 262  
Rzepka, K. 96  
S, H. 116  
Sadeq, S. M. A. 275  
Sadowski, J. 172  
Saeed, M. A. 49  
Sagdoldina, Z. 130  
Sahraoui, B. 45  
Sahul, M. 120  
Sajid, M. 68  
Sakamoto, T. 270  
Sala, L. 269, 296, 209  
Saltykov, D. 136  
Salvador, M. 217  
Sameer, S. 24  
Samilyk, A. 122  
Samoilov, O. 284, 231  
Sanij, F. D. 90  
Santana-Otero, A. 217  
Sarnatskaya, V. 279, 283  
Sarwar, M. 144  
Satbayeva, Z. 124, 133  
Sato, T. 125  
Satrapinskyy, L. 186, 211  
Saulenko, K. 279  
Savranguler, E. N. 178  
Scalise, E. 14  
Scepka, T. 174  
Schirinzi, G. 280  
Schlichtholz, A. 64  
Schlichtholz, K. 64, 87  
Schmoranzner, D. 220  
Schröder, S. 210  
Schweizer, M. R. 164  
Schönhense, G. 172  
Sedyh, O. 278, 288  
Selmani, A. 272  
Semenova, O. 257  
Sementsov, Y. 33, 34

- Seminko, V. 278, 290, 284, 285, 231, 232, 288  
Sencha-Hlevatska, K. 33  
Serdeha, I. 146  
Serha, R. 160  
Shablenko, V. 170  
Shah, M. 28  
Shah, R. 28  
Sharma, A. 298, 183  
Shchokotova, O. 62  
Shevchuk, L. 148  
Shigekawa, H. 179  
Shima, T. 154  
Shimizu, T. 277  
Shiratani, M. 105  
Shkurdoda, Y. 185, 186, 43, 44, 136  
Shlapa, Y. 173, 279  
Shoji, Y. 113  
Shpetnyy, I. 186, 211  
Shrivastav, V. 37  
Shtanko, O. 187, 191, 196  
Shtepa, D. 131  
Shubin, P. 135  
Shvets, S. 186  
Shvets, U. 186  
Sijo, S. 24  
Sikiric, M. 123  
Silhanek, A. 198, 199  
Simka, W. 135  
Singh, J. 287  
Singh, N. 22, 24  
Sirakoulis, G. C. 293  
Siuzdak, K. 15, 71  
Sivakumar, S. 95, 23  
Skakalova, V. 13  
Skorvankova, K. 25  
Skrypnichuk, V. 35  
Skryshevsky, V. 268, 289  
Skydanenko, M. 281  
Slaboseviciute, G. 212  
Slavin, A. 214  
Smokal, V. 31  
Smortsova, Y. 147  
Sobetskii, A. 139  
Sobol, K. 208, 68  
Sobti, A. 27  
Sokoliuk, D. 47  
Solař, P. 25  
Solodovnyk, O. 61  
Soni, A. 18  
Sotnyk, I. 175, 191  
Sousani, S. 174, 180  
Stabnikova, O. 132  
Stanković, A. 272  
Stasiuk, O. 32  
Stastny, M. 261, 262, 248, 263  
Staño, E. 211  
Strmcnik, D. 91  
Strunskus, T. 210  
Stępień, M. 113  
Subotic, N. 179  
Suess, D. 169  
Sugihara, M. 210  
Sukhodub, L. 60  
Sulka, G. D. 96  
Sullivan, C. 166  
Sung, H. 109, 17  
Synak, A. 64  
Szatny, M. 127  
Szeluga, U. 47  
Sümer, İ. E. 223  
Taboukhat, S. 45  
Takahashi, M. 179  
Takeuchi, O. 179  
Talaikis, M. 184  
Talipova, A. 139  
Tang, H. 34  
Tapajna, M. 143  
Tataryn, N. 195, 172  
Taşçılar, N. E. 228, 188  
Tepavcevic, S. 89  
Tereshina-Chitrova, E. 167  
Terets, M. 33  
Teslyuk, I. 45  
Thaha, F. H. 22  
Tkach, O. 172  
Tomita, S. 153  
Tompriš, I. 293  
Topchylo, A. 268, 289  
Tovstenko-Zabelin, M. 276  
Tovstolytkin, O. 173  
Tsunashima, R. 112  
Turabekov, E. 134  
Turos, A. 142  
Turutanov, O. G. 149  
Tyberkevych, V. 214  
Tymoshenko, O. 249  
Tóbbik, J. 174  
Túnica, M. 14  
Ullah, A. 28  
Umetsu, R. Y. 168  
Ushkalov, V. 249  
Učakar, A. 272  
Vadlamudi, S. G. 143  
Vagner, I. 256  
Vaicekauskaitė, E. 215  
Vaisocherová-Lísalová, H. 138  
Valdez, F. J. S. 258  
Valesia, A. 280  
Valášková, M. 138  
Van Bael, M. 199  
Van de Vondel, J. 198, 199  
Van Zomeren, A. 217  
Varga, M. 143  
Varlam, M. 256, 297  
Varlamov, A. 9  
Varvarin, M. 259  
Vasylechko, V. 148  
Vasylyk, Y. 264  
Vedel, D. 29, 32  
Veintemillas-Verdaguer, S. 217  
Velotta, R. 74  
Verma, A. 230  
Vervoort, S. 199  
Vetrova, I. 174, 203  
Vidiš, M. 211  
Viera, M. 239  
Vinnikov, M. 41  
Virt, I. S. 119  
Virych, P. 31, 279, 283  
Vladimirova, T. 264  
Vodeb, O. 91  
Voicu, R. C. 53  
Volavka, D. 90  
Volek, T. 236  
Volk, I. 43, 136  
Voloshinovskii, A. 148  
Vorobiov, S. 185, 186, 90  
Voss, L. 104  
Vygovska, L. 249  
Wakabayashi, Y. 105  
Waleng, N. J. 238  
Wang, D. 33, 34  
Wang, H. 221  
Wang, X. 152  
Watras, A. 274  
Weinert, M. 151  
Wiglusz, R. 274  
Winkowska-Struzik, M. 101, 102  
Wintz, S. 157  
Wojtas, F. 50  
Wosinski, T. 172  
Wozniak, W. 144  
Wróbel, M. 127, 113, 114  
Wu, M. 33  
Wu, W. 206  
Xu, R. 161  
Yadgarov, L. 257  
Yamada, T. K. 108  
Yamamoto, T. 105  
Yamashita, T. 201  
Yanko, I. 50, 61  
Yarıçi, İ. 176  
Yaroshenko, K. 247  
Yastrubchak, O. 195, 172  
Yefimova, S. 284, 285, 231, 232  
Yeow, J. 207  
Yeshchenko, M. 31  
Yeshchenko, O. 224, 218, 254, 242  
Yu, M. 85  
Yurchenko, O. 121  
Yurkova, A. 52  
Zaderko, A. 268, 289  
Zaghrioui, M. 20  
Zahorodna, V. 77  
Zahorodnia, S. D. 276  
Zaika, V. 146  
Zak, A. 12, 234  
Zapol, P. 92  
Zaraska, L. 16  
Załęski, K. 15  
Zdurienčík, M. 143  
Zhang, Z. 120  
Zharnikov, M. 113  
Zhelezny, V. 265  
Zheltonozhskaya, T. 276  
Zhu, J. 21  
Zhydenko, I. 59  
Zhytskyi, A. 229  
Zobelli, A. 14  
Zoladek, S. 99, 97  
Zosimov, R. 204  
Zozulya, G. 35

Zraichenko, O. V. 149  
Zvirzdine, G. 212  
Zápražný, Z. 203, 143  
Çoşut, B. 70  
Ömür, Y. Ö. 228, 188  
Čerkesa, A. 260  
Čundrle, J. 263

Đurina, P. 211  
Świerkula, A. A. 16  
Şahin, F. 223  
Šamožil, T. 220  
Škriniarová, J. 227  
Škute, N. 258, 260  
Šoltýs, J. 174, 203, 180

Šćepanović, S. 194  
Šćepka, T. 203, 180  
Št'atná, J. 25  
Živković, K. 272  
Žukauskas, Š. 68