The 4th Serbian Conference on Materials Application and Technology - SCOM

National conference with international participation

BOOK OF ABSTRACTS

Editor:
Prof. Dr. Miroslav Dramićanin
Centre of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade

Published and printed by: Društvo za razvoj nauke Srbije, Belgrade

Print run: 50

ISBN-978-86-904450-5-9
CIP 66.017/.018(048)(0.034.2)
620.1:66.017/.018(048)(0.034.2)

October 2025, Belgrade, Serbia

SCOM 2025

The 4th Serbian Conference on Materials Application and Technology

BOOK OF ABSTRACTS

October 15th – 17th 2025. Belgrade, Serbia

Dear Colleagues and Friends,

It is our great pleasure to welcome you to the second Serbian Conference on Materials Application and Technology - SCOM2025. The conference is jointly organized by the Society for the Science Development of Serbia and the Vlatacom Research and Development Institute. With a focus on cutting-edge materials design, fabrication, and integration as well as ground-breaking materials-based technologies, SCOM2025 is the new home for all materials-related technological research. This conference will highlight the most recent advancements in the field of materials technology and application aiming to bridge the gap between researchers working on materials and technology users. Energy, healthcare, electronics, optics, microfluidics, sensors, food safety, and other topics will be covered. This year, four tutorial lectures, four invited lectures, and nine oral presentations on the following topics will be given: Nanomaterials, Biomaterials, Optical and Photonic Materials, Materials for energy production and storage, Chemo/Bio/Physical Engineering, Photocatalysis, Green technologies, Sensor materials and technologies, Materials synthesis and processing.

We anticipate that SCOM2025 will be fruitful in terms of scientific exchange and that it will strengthen existing collaborations among participants while also fostering future ones. We would like to thank various organizations for their financial assistance.

Organizers of the SCOM2025 wish you a nice time during the conference in Belgrade!

Conference Chairperson

Prof. Dr. Miroslav D. Dramićanin

Our sponsors:

Република Србија

МИНИСТАРСТВО НАУКЕ,
ТЕХНОЛОШКОГ РАЗВОЈА И
ИНОВАЦИЈА

SUPERLAB®
Your lab – Our passion

CEI
CENTRAL EUROPEAN INITIATIVE

Program and Advisory Board and Reviewers:

Dr. Željka Antić
Centre of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade

Prof. Dr. Miroslav Dramićanin
Centre of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade

Prof. Dr. Thomas Thundat
University at Buffalo Department of Chemical and Biological Engineering, Buffalo, New York, USA

Prof. Dr. Mikhail Brik
Centre of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade

Dr. Alessandra Toncelli
Università di Pisa, Pisa, Italy

Dr. Lukasz Marciniak
Institute of Low Temperature and Structure Research Polish Academy of Sciences, Poland

Dr. Kumar Prashanthi
University of Alberta, Edmonton, Canada

Dr. Chong-Geng Ma
Chongqing University of Posts and Telecommunications, Chongqing, China

Prof. Dr. Anatolijs Šarakovskis
Laboratory of Spectroscopy, Institute of Solid State Physics, University of Latvia, Riga, Latvia

Prof. Dr. Vladimirs Pankratovs
Laboratory of Spectroscopy, Institute of Solid State Physics, University of Latvia, Riga, Latvia

Dr. Lei Zhou
School of Chemical Engineering and Technology, Sun Yat-sen University (Zhuhai Campus), Zhuhai City, China

Prof. Dr. Đorđe Veljović
Faculty of Technology and Metallurgy, University of Belgrade

Dr. *Tamara Gavrilović*
Centre of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade

Dr. *Milica Maričić*
Centre of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade

Dr. *Miroslav Perić*
Vlatacom Research and Development Institute, Belgrade, Serbia

Dr. *Dragana Perić*
Vlatacom Research and Development Institute, Belgrade, Serbia

Dr. *Aleksej Makarov*
Vlatacom Research and Development Institute, Belgrade, Serbia

Organizing committee:

Dr. Željka Antić
Centre of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade

Dr. Milica Maričić
Centre of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade

Dr. Ljubica Đačanin Far
Centre of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade

Dr. Bojana Milićević
Centre of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade

Dr. Mina Medić
Centre of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade

Dr. Tamara Matić
Faculty of Technology and Metallurgy, University of Belgrade

Katarina Milenković
Centre of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade

Anđela Rajčić
Centre of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade

FIRST-PRINCIPLES CALCULATIONS FOR INTRINSIC AND EXTRINSIC DEFECTS IN SOLIDS: METHODOLOGY AND CASE STUDIES

Chong-Geng Ma (0000-0001-8090-1738)
School of Integrated Circuits & CQUPT-BUL Innovation Institute, Chongqing University of Posts and Telecommunications, No.2 Chongwen Road, Nan'an District, Chongqing 400065, China, cgma.ustc@gmail.com

This lecture provides a comprehensive overview of the speaker's research on the first-principles design of novel luminescent materials doped with lanthanide, transition-metal, and ns^2-type ions [1]. It begins with an introduction to density functional theory (DFT) and its application in modeling the geometrical and electronic structures of pristine host materials. The discussion then systematically progresses to the modeling of intrinsic and extrinsic defects: we first detail DFT-based methodologies for investigating defects in their ground state, and further advance to approaches for capturing their excited-state properties [2,3]. Through selected case studies, the lecture demonstrates the successful application of these methods and underscores the reliability of our theoretical framework, which shows excellent agreement with experimental observations. Finally, we conclude that the proposed theoretical strategies offer a powerful and predictive guide for the discovery and rational optimization of high-performance phosphors [4].

Acknowledgements: This work was financially supported by the National Natural Science Foundation of China (Grant Nos. U24A2056, 12274048, and 52161135110), and China-Serbia Intergovernmental Science and Technology Cooperation Program (Grant No. 2024[7]/6-10).

References:

[1] Y.S. Wang, B.B. Lou, P.P. Dang, G.D. Zhang, Y.J. Wan, L. Tian, H.Z. Lian, Z.Y. Hou, C.-G. Ma, G.G. Li, J. Lin, Angew. Chem. Int. Ed. 64 (2025) e202416021.
[2] A. Zunger, O.I. Malyi, hem. Rev. 121 (2021) 3031−3060.
[3] A. Hellman, B. Razaznejad, B.I. Lundqvist, J. Chem. Phys. 120 (2004) 4593-4602.
[4] K. Han, J. Qiao, S. Zhang, B. Su, B. Lou, C.-G. Ma, Z. Xia, Laser Photonics Rev. 17 (2022) 202200458.

HOW TO EFFECTIVELY IMPROVE THE DESIRED PROPERTIES OF ENERGY HARVESTING MATERIALS?

Michal Piasecki (0000-0003-1040-8811)
Institute of Chemistry, Jan Dlugosz, University of Czestochowa, al. Armii Krajowej 13/15, 42-200 Czestochowa, Poland, m.piasecki@ujd.edu.pl

It is well known that the changes of chemical composition, structure, temperature, stress or strain caused by external pressure or temperature influence structural, optical, magnetic, thermoelectric or super-conducting properties of solids. Band gap engineering through the modification of the composition is an effective method to adjust electronic and optical properties of such mixed compounds or composites to meet special requirements for its efficient operation in a particular application. Thanks to these phenomena, constructed (transformed) materials, demonstrating totally different properties, than are desired in nature. We will focus on the influence of composition (non-stoichiometry, high configurational entropy, structure defects), size, temperature or pressure on the structure, electronic and luminescence properties. Finally, examples improved (or tuned) promising materials interesting for superconductivity, thermoelectricity, dosimetry, lighting, remote temperature or pressure sensing will be discussed. Rapid advances in reliable computational DFT-based methods have paved a broad way towards increasing importance of so-called “theoretical experiments”, when thoroughly performed calculations replace or forego experiments and even predict unknown materials and their properties. In present talk we also discuss the opportunities (and disadvantages) of quantum chemical calculations towards searching for new efficient materials for energy harvesting.

T-3

APPLICATION OF X-RAY PHOTOELECTRON SPECTROSCOPY FOR VERIFICATION OF DFT BAND-STRUCTURE CALCULATIONS OF SOLIDS

Oleg Khyzhun (0000-0002-2403-8607)[a,b]
[a] *Jan Dlugosz University in Czestochowa, Poland*
[b] *Frantsevich Institute for Problems of Materials Science, National Academy of Sciences of Ukraine, Kyiv, khyzhun@ukr.net*

During the lecture, the main advantages of X-ray photoelectron spectroscopy (XPS) for studies of the electronic structure of solids will be considered. Peculiar features of binding energy scale calibrations for XPS spectrometers and taking into account surface charging effects in solids will be discussed. Peculiarities of possible techniques for verification of density functional theory (DFT) band-structure calculations of solids will be given. We will also discuss application of XPS in combination with other techniques, e.g., X-ray emission spectroscopy (XES), X-ray absorption spectroscopy (XAS), ultraviolet photoelectron spectroscopy (UPS), for probing theoretical calculating data regarding total density of states (TDOS) and partial densities of states (PDOS) of different kinds of materials: metals, semiconductors, insulators. Application of modern synchrotron facilities for studying XPS, XES, and XAS spectra will be also considered.

T-4

INTRODUCTION TO DETERMINING CRYSTAL STRUCTURE BY X-RAY DIFFRACTION

Volodymyr Pavlyuk (0000-0003-1893-2706)[a,b]
[a]*Institute of Chemistry, Jan Dlugosz, University of Czestochowa, al. Armii Krajowej 13/15, 42-200 Czestochowa, Poland*
[b]*Department of Inorganic Chemistry, Ivan Franko Lviv National University, Kyryla, and Mefodiya str., 6, 79005, Lviv, Ukraine, vpavlyuk2002@yahoo.com*

During the lecture, the main methods of studying the crystal structure of materials using X-ray diffraction will be considered. Modern approaches to studying the crystal structure using both methods, powder and single crystals, will be considered. We will also discuss modern software packages for both groups of methods, in particular, such as SHELX, CSD and FullProf. Special attention will be paid to the analysis of the obtained data and the generation of CIF files. The features of submitting structural data to databases and preparing publications in CIF format will be considered.

DATA-DRIVEN THERMOMETRY ON Mn^{5+} DOPED $Ca_6Ba(PO_4)_4O$ PHOSPHOR

Zoran Ristić (0000-0002-1854-284X), Sanja Kuzman (0000-0001-9657-9122), Miroslav Dramićanin (0000-0003-4750-5359)
Center of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia
risticz@vin.bg.ac.rs

In this study, several data-driven approaches were applied to a single dataset of Mn^{5+} doped $Ca_6Ba(PO_4)_4O$ temperature-dependent luminescence emission spectra to improve the temperature resolution of this Mn^{5+} based luminescent thermometer. In addition to conventional approaches in luminescent thermometry such as luminescence intensity ratio (LIR) and band shift analysis, multiple linear regression (MLR) and principal component analysis (PCA) methods were also applied. MLR forms a linear combination of conventional readouts to create a new one to be used as a thermometric parameter. PCA is a technique for linear dimensionality reduction that reorients spectroscopic data onto a new coordinate system so that the principal components with the greatest variance become readily identifiable and used as a thermometric parameter. Since all these methods were applied to a single dataset, a direct comparative comparison was facilitated. PCA demonstrated superior temperature resolution compared to traditional methods and MLR. The average resolution was 0.135 K in the 290 K to 375 K temperature range and 0.074 K in the physiological range (303 K to 318 K).

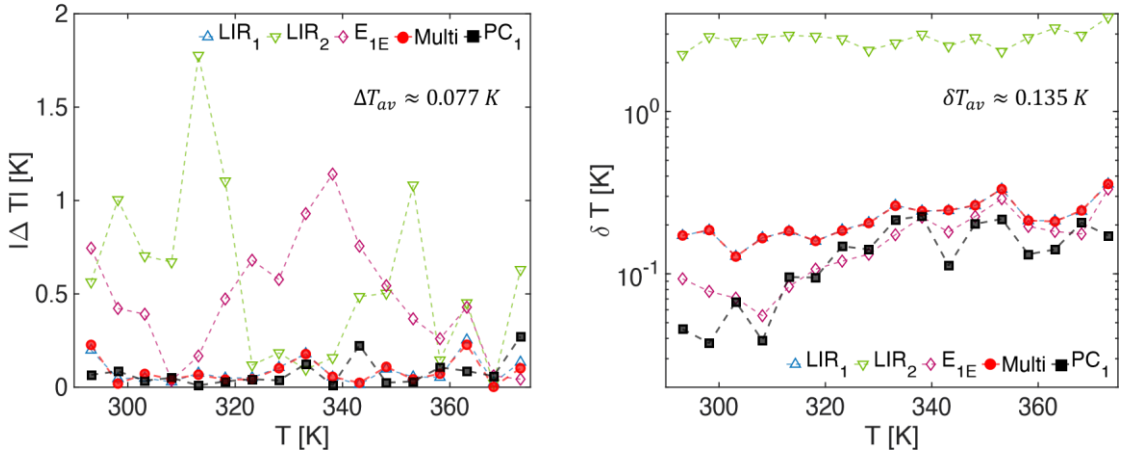


Figure1. Temperature dependent accuracy ($\Delta T(T)$) and resolution ($\delta T(T)$) for different applied methods

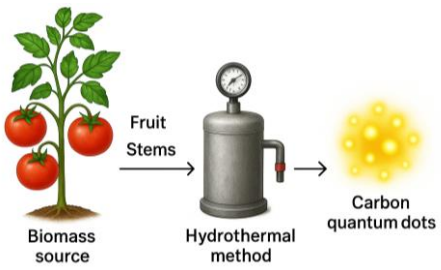
Acknowledgment:
This research was supported by the Science Fund of the Republic of Serbia, #GRANT No 7017, TECHNOLOGY FOR REMOTE TEMPERATURE MEASUREMENTS IN MICROFLUIDIC DEVICES – REMTES. Authors acknowledge funding of the Ministry of Science, Technological Development, and Innovation of the Republic of Serbia under contract 451-03- 66/2024-03/ 200017.

BIOMASS-DERIVED CARBON QUANTUM DOTS: STRUCTURAL INSIGHTS AND PHOTOLUMINESCENCE FROM TOMATO SOURCES

Jovana Periša (0000-0002-4683-0603)[1], Bojana Milićević (0000-0003-2870-2728)[1], Jan Hočevar (0009-0000-7725-4453)[2], Jernej Iskra (0000-0001-6340-3577)[2], Boštjan Genorio (0000-0002-0714-3472)[2], Darja Lisjak (0000-0003-4154-4592)[3], Miroslav D. Dramićanin (0000-0003-4750-5359)[1], Jelena Papan Djaniš (0000-0002-1743-5997)[1,2*]

[1] *Centre of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade, 11351 Belgrade, Serbia*
[2] *Faculty of Chemistry and Chemical Technology, University of Ljubljana, 1000 Ljubljana, Slovenia, Jelena.PapanDjanis@fkkt.uni-lj.si*
[3] *Department for the Synthesis of Materials, Jožef Stefan Institute, 1000 Ljubljana, Slovenia*

Carbon quantum dots (CQDs) are a new class of nanomaterials known for their bright fluorescence, biocompatibility, and potential in sustainable technologies[1]. In this study, we demonstrate the use of tomato biomass as a natural and renewable source for producing CQDs. Tomatoes, one of the world's most cultivated crops, generate substantial amounts of processing waste, peels, and residues that often remain underutilized[2]. By converting this agricultural by-product into CQDs through a simple hydrothermal route, we highlight a strategy for biomass valorization that combines waste reduction with high-value nanomaterial production. The resulting CQDs displayed stable dispersibility in water and exhibited tunable fluorescence, with bright emission observed under ultraviolet light. Beyond their optical performance, this work underscores the broader environmental and economic potential of transforming food waste streams into functional nanomaterials. Such an approach supports circular economy practices, demonstrating that agricultural residues can be upgraded into advanced materials for applications in sensing, imaging, and green optoelectronics.



Acknowledgements: The authors gratefully acknowledge the financial support from the Slovenian Research Agency (ARIS) – research core funding grants P1-0134, P2-0423, and P1-0418, research project J2-50061, and Young Researcher Grant to J.H.). The authors from the Vinča Institute of Nuclear Sciences would like to acknowledge funding from the Ministry of Science, Technological Development, and Innovation of the Republic of Serbia under contract 451-03-136/2025-03/200017.

References:

1 Ahuja, V. *et al*. Quantum dot synthesis from waste biomass and its applications in energy and bioremediation. *Chemosphere* **293** (2022).
2 Almeida, P. V., Gando-Ferreira, L. M. & Quina, M. J. Tomato Residue Management from a Biorefinery Perspective and towards a Circular Economy. *Foods* **13**, 1873 (2024).

CURRENT TRENDS IN THE DEVELOPMENT OF DENTAL COMPOSITES WITH ENHANCED OPTICAL PROPERTIES

Dragica Manojlović (0000-0002-9653-4255)
University of Belgrade, School of Dental Medicine, Department of Restorative Odontology and Endodontics, Rankeova 4, 11000 Belgrade, Serbia, dragica.manojlovic@stomf.bg.ac.rs

The purpose of this lecture is to emphasize current trends in the development of composite materials with enhanced optical properties. The quest for superior aesthetic results in restorative dentistry has resulted in significant advancements in resin-based composite technology. Recently, these advancements have concentrated not only on accurately replicating the natural appearance of teeth but also on streamlining shade selection and clinical procedures.

Modern materials have been increasingly optimized through advanced silanization techniques to improve the interface between fillers and the resin matrix. This has enabled the formulation of materials with higher filler content while maintaining low viscosity, particularly in injectable composites suitable for the injection molding technique in the manufacture of composite veneers. This minimally invasive approach preserves tooth structure while delivering predictable and long-lasting esthetic results. Additionally, filler particles with carefully controlled size, shape, and varying refractive indices are being incorporated within a single material to maximize the so-called "chameleon effect." This effect enhances the material's ability to blend with surrounding dental tissues, regardless of the underlying tooth shade.These innovations have laid the groundwork for the development of single-shade and universal composites with simplified shade systems, where one core shade can adapt to several within the VITA shade guide. A notable example is G-ænial A'CHORD®, which uses just five core shades to cover all 16 VITA shades.

As a result of these developments, modern composites now offer improved optical properties that closely resemble natural dental tissues, along with favorable mechanical strength, excellent polishability, and user-friendly handling — all while streamlining restorative procedures.

SOLID LIPID-METAL NANOPARTICLES FUNCIONALIZED BY AMINO ACIDS

Anamarija Abu el Rub (0000-0001-9164-3965)[1], Anđela Rajčić(0009-0002-8242-7050)[1], Sara Stojanović (0009-0009-5627-6667)[2], Tamara Djukić (0000-0001-5897-6354)[3], Vladimir Djoković (0000-0001-8237-1101)[1], Radovan Dojčilović (0000-0002-3478-8268)[1]

[1] *Centre of excellence for photoconversion, Department of Radiation Chemistry and Physics, Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia, anamarija.abuelrub@vin.bg.ac.rs*

[2] *Faculty of Biology, University of Belgrade, Belgrade, Serbia*

[3] *Innovation Center, Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia*

Lipid nanoparticles are one of the most studied nano-systems for their potential use in medicine today. Their advantages include biocompatibility, size tuneability, charge and surface modifications, and excellent drug loading and delivery. Metal nanoparticles have multiple applications in biomedicine, being studied as contrast, theranostic and cytotoxic agents. Possibility of combining these systems, along with funcionalization of both metal and lipid nanoparticles, allows for building complex multipurpose nano-systems with novel properties. We have used electrospray method to synthesize solid lipid-metal nanoparticles comprising stearic acid as the lipid carrier and palladium nanoparticles functionalized with different amino-acids as metalic component. The nanosystems were characterized by UV-VIS and fluorescence spectroscopy, as well as by using XRD, DLS, fluorescence and electron microscopy. By studying the parameters such as lipid concentration, electrospray voltage and flow rate, the nano-systems were optimized in therms of their size and stability. The lipid nano-systems combined with palladium nanoparticles show better capability for retaining the trapped amino-acids and show promising properties for further studies as drug delivery agents.

References:

[1] It may all come down to the mechanisms of nanoparticle delivery. Nat Rev Bioeng 2, 193 (2024)
[2] L. Xu, X. Wang, Y. Liu, G. Yang, R.J. Falconer, C.-X. Zhao, Lipid Nanoparticles for Drug Delivery, Adv. NanoBiomed Res. 2 (2022) 2100109

PHOTOCATALYTIC AND ANTIMICROBIAL PROPERTIES OF RARE-EARTH-DOPED BiOCl

Anđela Rajčić (0009-0002-8242-7050), Mina Medić (0000-0001-8950-2426), Tamara Gavrilović (0000-0002-6581-2662), Katarina Isaković (0009-0007-7150-706X), Vesna Lazić (0000-0001-6440-6577), Miroslav Dramićanin (0000-0003-4750-5359)
University of Belgrade, Vinča Institute of Nuclear Sciences, National Institute of Republic Serbia, P.O. Box 522, Belgrade 11001, Serbia, andjela.rajcic@vin.bg.ac.rs

The excessive use of pharmaceuticals and textile dyes contributes significantly to water pollution, posing severe risks to human and environmental health. To overcome these difficulties, photocatalysis has become a viable, effective, and economical way to break down organic contaminants. In this study, BiOCl:Pr (BiOCl) 2D nano-microsheets were synthesized via a coprecipitation method and characterized using XRD, SEM, TGA, BET, and UV-VIS analyses. XRD results confirmed the tetragonal BiOCl structure (space group P4/nmm, 129)***(Figure 1)***. The photocatalytic performance was investigated through the visible-light-activated degradation of Acid Orange 7 (AO7), and a kinetic analysis at varying initial dye concentrations was conducted to evaluate the corresponding photodegradation rates. Pr doping was found to significantly enhance the photocatalytic and antibacterial properties of BiOCl. The results demonstrated that 3% Pr-doped BiOCl exhibited markedly enhanced photocatalytic efficiency compared to pure BiOCl. Furthermore, the material exhibited pronounced antibacterial activity under visible light, highlighting its potential as a stable and multifunctional photocatalyst for the removal of organic pollutants and microbial contaminants from aqueous systems**.**

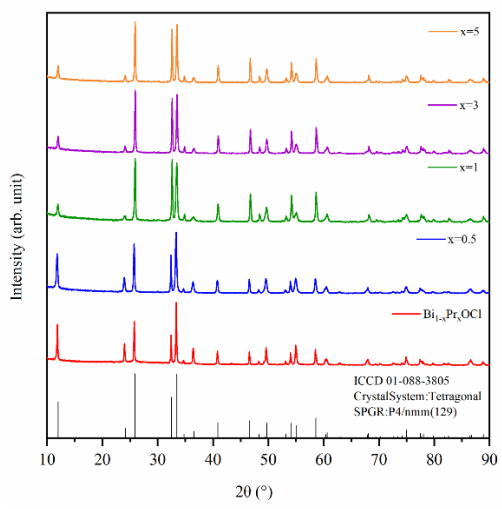


Figure 1. XRD patterns of the Pr^{3+} doped BiOCl samples

Acknowledgment:
Authors acknowledge funding of the Ministry of Science, Technological Development, and Innovation of the Republic of Serbia under contract 451-03- 66/2024-03/ 200017.

OPTIMISATION OF TITANIUM DIOXIDE PHOTOCATALYTIC EFFICIENCY WITH LIGNIN DERIVED CARBON QUANTUM DOTS

Azmat Ullah (0009-0009-5345-1001)[a], Andraž Šuligoj (0000-0002-7971-1424)[a], Iskra Jernej (0000-0001-6340-3577)[a], Urška Lavrenčič Štangar (0000-0001-9652-2257)[a], Jelena Papan Djaniš (0000-0002-1743-5997)[a,b] *

[a] *Faculty of Chemistry and Chemical Technology, University of Ljubljana, Večna pot 113, SI-1000 Ljubljana, Slovenia, Azmat.Ullah@fkkt.uni-lj.si*

[b] *Centre of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade, 11351 Belgrade, Serbia*

Photocatalysis as a green technique is applied for water splitting, CO_2 conversion, pollutants degradation, and selective organic reactions [1]. It utilizes only a light source at room temperature to carry out catalysis. TiO_2 is used as a benchmark in photocatalysis due to its chemical stability, high oxidative capability, and relatively low cost [2]. Some problems *e.g.* wide band gap and smaller light absorption range, restrict practical applications of TiO_2. TiO_2 is functional as a photocatalyst under ultraviolet (UV) light but inactive under visible light. UV light is only 5% of sunlight [3]. So, it is not desirable to use UV light for photocatalysis. In this study, the photocatalytic efficiency of TiO_2 under visible light was optimized by preparing its hybrid with lignin-derived carbon quantum dots (CQDs). CQDs from spruce lignin were synthesized through the hydrothermal synthesis method. Lignin is the second most abundant natural biopolymer after cellulose in terrestrial ecosystems and a byproduct of the paper industry [4]. The synthesized CQDs were coupled with TiO_2 to get CQDs/TiO_2 hybrid (**Figure 1**). TiO_2 and TiO_2 hybrid (3%CQDs50/TiO_2) were used for the photodegradation of a five-pharmaceutical mixture in visible light (400-700nm), and the efficiencies of both photocatalysts were compared. It was found that CQDs synergistically coupled with TiO_2 enhanced the photocatalytic activity of TiO_2 under visible light.

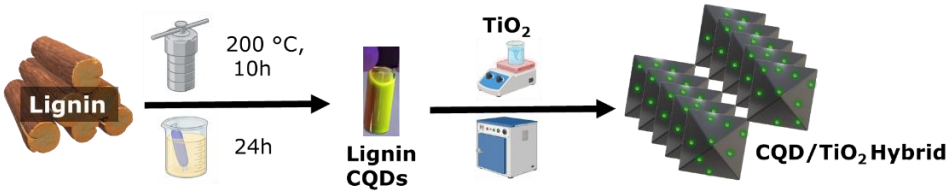


Figure 1. Preparation of CQDs/TiO_2 hybrid

Acknowledgement: The authors acknowledge the Slovenian Research Agency (ARIS) through research core funding grants P1-0134 and P1-0418, and research project J2-50061.

References:

[1] Y. Q. Yan *et al.*, "Recent Advances of CeO_2-Based Composite Materials for Photocatalytic Applications.," *ChemSusChem*, vol. 17, no. 14, pp. e202301778–e202301778, Mar. 2024.

[2] A. Velázquez *et al.*, "Benchmarking of photocatalytic coatings performance and their activation towards pollutants degradation," *Prog Org Coat*, vol. 147, p. 105856, Oct. 2020.

[3] B. L. Diffey, "Sources and measurement of ultraviolet radiation," *Methods*, vol. 28, no. 1, pp. 4–13, Sep. 2002.

[4] M. Ayyachamy *et al.*, "Lignin: untapped biopolymers in biomass conversion technologies," *Biomass Conversion and Biorefinery 2013 3:3*, vol. 3, no. 3, pp. 255–269, Jun. 2013

O-4

ASSESSMENT OF THE TOXICITY AND GERMICIDAL ACTIVITY OF $Y_2SiO_5:Pr^{3+}$ AND $La(PO_3)_3:Pr^{3+}$ COMPOUNDS AGAINST *Escherichia coli*

Cristina Mosoarca (0000-0001-9969-4900)[a], Radu Banica (0000-0002-9435-2837)[a], Miroslav Dramicanin (0000-0003-4750-5359)[a,b], Zeljka Antic (0000-0002-7990-2001)[a,b], Ramona Vetési[c]

[a]*National Institute of Research and Development for Electrochemistry and Condensed Matter, Str. Dr. A. Păunescu Podeanu nr.144, 300569 Timisoara, Romania, mosoarca.c@gmail.com*

[b]*Centre of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences—National Institute of the Republic of Serbia, University of Belgrade, Mike Petrovi12-14, 11000 Belgrade, Serbia;*

[c]*Water Quality Control Laboratory, Aquatim S.A., Intrarea Carului 18, 307200, Timisoara, Romania*

Since ultraviolet C (UVC) radiation can damage microorganisms' DNA, it is frequently used in antimicrobial applications to render bacteria, viruses, and other pathogens inactive. In order to decontaminate water, food items, and other environmental surfaces, UVC-based treatments are essential. However, the high cost, energy consumption, and material limitations of conventional UVC sources frequently limit their use. In this regard, blue-to-UVC upconversion (UC) has become a viable method for utilizing affordable and accessible blue-light sources for antimicrobial and associated uses. This method provides a flexible platform for innovative disinfection technologies by enabling the localized generation of germicidal UVC photons from low-energy blue excitation.

Because of their special optical characteristics and chemical stability, rare-earth-doped inorganic phosphors are especially well-suited for UC-based antimicrobial applications.

In the present work, the germicidal performance of $Y_2SiO_5:Pr^{3+}$ and $La(PO_3)_3:Pr^{3+}$ powders was evaluated against the ATCC 8739 strain of E. coli by employing two distinct experimental protocols. Following this initial screening, the less toxic compound was incorporated into $Y_2SiO_5:Pr^{3+}$/PDMS composite membranes, and the germicidal effect of these membranes was investigated under blue-light excitation of the phosphor.

The results reveal that $La(PO_3)_3:Pr^{3+}$ exhibits noticeably higher toxicity toward E. coli than $Y_2SiO_5:Pr^{3+}$. Composites containing $Y_2SiO_5:Pr^{3+}$ demonstrate a moderate bactericidal efficiency attributable to UVC emission generated through the up-conversion process.

Acknowledgements: This study was supported by Romania's National Recovery and Resilience Plan, PNRR [project grant number C9-I8-28/FC 760107/2023].

O-5

NEXT-EDLC: CARBON-BASED ELECTRODE DEVELOPMENT FOR HIGH-PERFORMANCE SUPERCAPACITORS

Daniel M. Mijailović (0000-0003-1977-8325)[1], Miroslav Perić (0000-0002-7945-5571)[2], Dragana Perić (0000-0002-2556-8212)[2], Djordje T. Janaćković (0000-0002-8291-4345)[1], Petar S. Uskoković (0000-0001-9543-1732)[1]

[1]*Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, 11120 Belgrade, Serbia dmijailovic@tmf.bg.ac.rs*

[2]*Vlatacom Institute of High Technology, Milutina Milankovica 5, 11070 Belgrade, Serbia*

The NEXT-EDLC project targets the development of next-generation electrochemical double-layer capacitors (EDLCs) with improved energy density, power delivery, and scalability. Electrode formulations were systematically optimized for both aqueous and organic electrolyte systems. Activated carbon was combined with conductive additives (carbon black and carbon nanotubes) and tailored binders (CMC/SBR for aqueous, PVDF for organic) to produce uniform, crack-free coatings on carbon-coated copper foil. Process refinements such as staged high-shear and vacuum mixing, doctor-blade coating, controlled drying, and calendaring resulted in electrodes with excellent adhesion and mechanical flexibility. Symmetric CR2032 coin cells with 1 M KOH demonstrated specific capacitances between 50 and 60 F g^{-1}, nearly ideal capacitive CV profiles, and robust stability, with carbon nanotubes-enhanced formulations exhibiting superior high-rate retention compared to carbon black-only electrodes. These results highlight that optimized electrode architecture and process engineering can significantly improve capacitance, reduce internal resistance, and enhance rate capability. The project has identified the most promising formulations for scale-up and integration into pouch cells. The findings demonstrate the potential of engineered carbon-based electrodes to advance EDLC performance, bridging laboratory prototypes and practical applications in fast-charging, durable energy storage systems.

NOVEL HYBRID NANOMATERIALS AS NIR LIGHT-DRIVEN NANOMOTORS FOR BIOMEDICAL APPLICATIONS

Danijela Danilović (0000-0001-8402-1850)[a], Jelena Pajović (0000-0002-3644-0118)[b], Anamarija Abu el Rub (0000-0001-9164-3965)[a], Vladimir Djoković (0000-0001-8237-1101)[a], Biljana Ristić (0000-0002-7255-6556)[c], Tijana Maric (0000-0002-6847-251X)[d], Dušan K. Božanić (0000-0001-8246-9635)[a]

[a]*Center of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences–National Institute of the Republic of Serbia, University of Belgrade, P.O. Box 522, Belgrade 11001, Serbia, danijelad@vin.bg.ac.rs, anamarija.abuelrub@vin.bg.ac.rs, djokovic@vin.bg.ac.rs, bozanic@vin.bg.ac.rs*

[b]*University of Belgrade, Faculty of Physics, Studentski trg 12, Belgrade 11001, Serbia, jelena@ff.bg.ac.rs*

[c]*Institute for Medical Research, National Institute of the Republic of Serbia, University of Belgrade, Dr Subotića 4, PO Box 39, 11000 Belgrade, Serbia, biljana.ristic@imi.bg.ac.rs*

[d]*Technical University of Denmark, Ørsted Plads, 2800 Kgs. Lyngby, Denmark, tijma@dtu.dk*

Nanomotors are hybrid nanosystems, usually with Janus morphology, composed of an active component that converts external energy into mechanical motion and a functional component. Light-driven nanomotors are most extensively studied because light is a controllable and reusable energy source. The propulsion of light-driven nanomotors relies on photocatalytic, photothermal, or photoisomerization processes occurring on the active component, which create a gradient along the particle, thus inducing propulsion in the opposite direction, as illustrated in Figure 1. Near-infrared (NIR) light–driven nanomotors hold significant potential for biomedical applications such as drug delivery, photothermal and photodynamic therapy, and imaging, since NIR light can penetrate the skin.

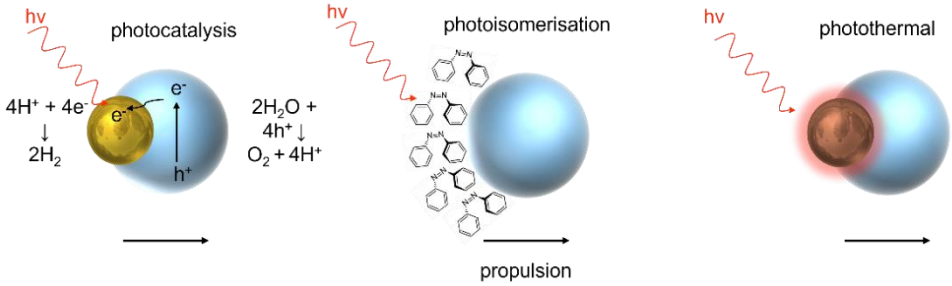


Figure 1. Light-induced movement of nanomotors

Here, we outline the procedures for the innovative fabrication of colloidal photothermal Janus nanomotors, which can be used for ballistic drug transport across cell membranes. These nanomotors are composed of mesoporous silica as a functional material, with photoactive components that are Ag-Ag_2S, Au, or $AgBiS_2$ nanoparticles that absorb light in the NIR region of the electromagnetic spectrum. The movement of nanomotors is examined using CARS microscopy, and the resulting particle tracks are analyzed with ImageJ TrackMate software.

Acknowledgements: This research is supported by the Science Fund of the Republic of Serbia, grant #275, Project - NIMPHA

References:

[1] X. Zeng, M. Yang, H. Liu. Nanoscale, 15 (2023) 18550.
[2] D. Danilović, T. Maric, D. K. Bozanic. Nano Research 18 (2025) 94907505.

O-7

ANALYSIS OF THE ELECTROMAGNETIC SHIELDING PROPERTIES OF GRAPHENE OXIDE COATED WITH PLATINUM NANOPARTICLES

Dušan N. Sredojević (0000-0003-2867-2047), Dejan Kepić (0000-0003-2777-6864), Anđela Stefanović (0000-0002-1092-5299), Svetlana Jovanović (0000-0002-2062-7527)
Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Mihajla Petrovića Alasa 12-14, 11351 Belgrade, Serbia, dusredo@vin.bg.ac.rs

Finding effective shielding material is becoming increasingly important as the market for electronic devices continues to grow and demands better protection against electromagnetic radiation. In this study, we used low-dose gamma irradiation to synthesize graphene oxide/platinum nanoparticle composites in a single step [1]. Pt NPs produced at irradiation dosages of 10 and 20 kGy were evenly distributed across the GO surface, with a significant fraction of particles up to 10 nm in size. Additionally, the sp^2 carbon structure of graphene was mostly restored using gamma irradiation. The structural and morphological characteristics of the generated composites were assessed using a variety of spectroscopic and microscopic methods, and the nature of the interactions between platinum clusters and graphene oxide sheets was investigated using density functional theory (DFT). Pt nanoparticles were formed due to the reduction of hexachloroplatinic acid by gamma irradiation, which also partially reduced graphene oxide (GO). The DFT calculations indicated that the electrical conductivities of GO and Pt NPs differ. This could lead to the redistribution of charges across the contact region, creating a conductive network at the interface that should enhance the EMI shielding capabilities of the composite. When measured at the X band, the shielding efficiency of the composites showed that 77% of the incident electromagnetic wave was blocked. A mismatch loss component was more prominent in the composite produced at a 20 kGy dosage due to the increased electrical conductivity caused by the irradiation.

Acknowledgements: This research was supported by the European Union's Horizon Europe Coordination and Support Actions programme under grant agreement No 101079151—GrInShield.

References:

[1] A. Stefanović, M. Yasir, G. Tobías-Rossell, S. S. Rojano, D. Sredojević, D. Kepić, D. Kleut, W. Saeed, M. Milović, D. Bajuk-Bogdanović, S. Jovanović, Molecules 30 (2025) 3579.

O-8

PREDICTION OF 5D LEVEL ABSORPTION WAVELENGTH IN INORGANIC HOSTS: RANDOM FOREST MODEL WITH SHAP PRIORITIZATION OF CANDIDATES

George-Daniel Dima[a,g] (0000-0002-4901-6340), Andrei Racu[a] (0009-0008-4058-7885), Mikhail Brik[a,b,c,d,e,f] (0000-0003-2841-2763), Željka Antić[a,b] (0000-0002-7990-2001), Miroslav D. Dramićanin[a,b] (0000-0003-4750-5359)

[a]*National Institute of R&D for Electrochemistry and Condensed Matter, INCEMC Timisoara, Romania, george.dima@upt.ro*

[b]*Centre of Excellence for Photoconversion, Vinća Institute of Nuclear Sciences –National Institute of the Republic of Serbia, University of Belgrade, Serbia*

[c] *Institute of Plasma Physics of the Czech Academy of Sciences, Czech Republic*

[d]*Faculty of Science and Technology, Jan Dlugosz University, Czestochowa, Poland*

[e]*Institute of Physics, University of Tartu, Estonia*

[f]*Academy of Romanian Scientists, Bucharest, Romania*

[g]*University Politehnica Timişoara, Timişoara, Romania*

This study presents the developed machine learning model for predicting the wavelength of the 5d level absorption in 5000 inorganic compounds doped with Pr^{3+} ions. The CIF (Crystallographic Information Files) structural dataset obtained from the Materials Project database was used for descriptor dataset formation. The data was initially collected using the MPRester Python library, followed by pre-processing, preliminary prediction, and refining of predictions. The RF (Random Forest) model was trained using a set of structural descriptors, including the bandgap, the distance *d(X... F)*, coordination number *CN*, angle ∠F–X–F, and lattice parameter *a,b,c* etc. The prediction results have a mean absolute error (MAE) of 2.42 nm. The model's interpretability was attained by SHAP (SHapley Additive exPlanations) values, both locally (per descriptor) and globally (per host). The beeswarm and partial dependency diagram indicate that the *bandgap* descriptor is potentially an important predictor related to the 5d level absorption value, succeeded by *d(X...F)*, *CN*, *∠F–X–F*, and *a*, all displaying predominantly impacts on the model's output value. To eliminate redundant information, filters were performed employing the Pearson correlation matrix, resulting in the suitable set of descriptors for the prediction refinement step. Utilizing the global SHAP value (the sum of absolute values per descriptor), the compounds were prioritized, and a potential list of candidates could be suggested by incorporating the criteria for alignment within the intended wavelength range. The results obtained guide host selection, decrease experimental effort, and indicate potential local structural adjustments.

Acknowledgements: The authors acknowledge the support of Romania's National Recovery and Resilience Plan - NRRP (PNRR), Project C9-I8-C28, and Contract 760107/2023.

References:

[1] G. Dima, A.V. Racu, C.G. Ma, A.M. Srivastava, Ž. Antić, M.D. Dramićanin and M.G. Brik, *J. Lumin*., vol. 286, 2025**,** 121359.

CELLULOSE-BASED HYDROGELS: EMERGING BIOMATERIALS FOR SUSTAINABLE APPLICATIONS

Jan Hočevar (0009-0000-7725-4453)[a], Boštjan Žener (0000-0002-0558-8080)[a], Romana Cerc Korošec (0000-0002-3486-5219)[a], Damjan Makuc[b], Janez Plavec (0000-0003-1570-8602)[a,b], Jernej Iskra (0000-0001-6340-3577)[a]

[a]*Faculty of Chemistry and Chemical Technology, University of Ljubljana, Večna pot 113, SI-1000 Ljubljana, Slovenia, Jernej.Iskra@fkkt.uni-lj.si*

[b]*Slovenian NMR Center, National Institute of Chemistry, Hajdrihova 19, SI-1000 Ljubljana, Slovenia*

The scarcity of resources, climate change and the accumulation of waste are increasingly urgent ecological challenges. Consequently, increasing attention is directed towards biomass, composed mainly of lignin, hemicellulose and cellulose. It is the most abundant biopolymer on earth and enables a range of chemical reactions to modify and form biomaterials [1]. These include cellulose hydrogels, which are three-dimensional, water-swollen polymer networks. Their ability to store large amounts of water, combined with softness, porosity and biocompatibility, makes them useful in medical, agricultural, pharmaceutical, food and textile applications [2]. Moreover "smart" hydrogels respond to pH, temperature, light, magnetic fields or electrical signals, offering promise for targeted drug delivery and biosensing [3]. Hydrogels can be synthesised by various physical and chemical cross-linking methods. In contrast to cellulose derivatives, cellulose is not soluble in common organic solvents, which poses an additional challenge in the synthesis of cellulose hydrogels.

This study investigates how the structure of bio-based crosslinkers influences the properties of cellulose hydrogels, focusing on alkyl chain length, crosslinker-to-cellulose molar ratio and the presence of free carboxyl groups. These structural parameters are expected to determine the flexibility of the polymer network, the pore size distribution and the swelling behaviour, which are crucial for the adaptation of hydrogels to specific applications.

To elucidate the structure–property relationships, we applied Fourier transform infrared spectroscopy (FTIR), solid-state nuclear magnetic resonance spectroscopy (NMR), thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC). This approach enabled direct correlation between synthetic parameters and material properties (Figure 1).

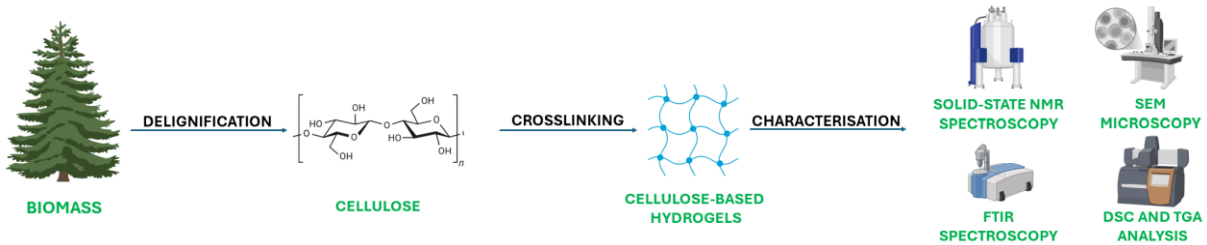


Figure 1. Path from cellulose to cellulose hydrogels and determination of their properties.

Acknowledgements: We thank the Slovenian Research and Innovation Agency (grant P1-0134) for funding this research.

References

[1] S.V. Vassilev, D. Baxter, L.K. Andersen, C.G. Vassileva, Fuel, 89 (2010), 913-933.
[2] X. Shen, J. Shamshina, P. Berton, G. Gurau, R.D. Rogers, Green Chemistry, 18 (2016), 53-75.
[3] H.M. El-Husseny, et al. Mater. Today Bio, 13 (2022), 100186.

O-10

HYDROGEN BINDING AND HYDROGEN CLEAVAGE ON SINGLE METAL-DECORATED CIRCUMCORONENES

Michal Malček (0000-0002-1920-1123), Ondrej Tkáč (0009-0008-7244-4029), Lukas Bucinsky (0000-0002-0190-3231)

[a] *Institute of Physical Chemistry and Chemical Physics, Faculty of Chemical and Food Technology, Slovak University of Technology in Bratislava, Radlinského 9, SK-812 37 Bratislava, Slovak Republic, michal.malcek@stuba.sk*

Graphene quantum dots, such as circumcoronenes (CCs), modified with transition metal atoms are nowadays extensively studied [1, 2]. In the presented work, an interaction between the hydrogen molecules and circumcoronenes decorated with single metal atoms (Sc, Ti, and V) is computationally investigated at the DFT level of theory. The studied systems show ability to bind H_2 molecules via two distinct ways: i) formation of η^2-coordination (Kubas interaction [3]); ii) dissociation of H_2 molecule resulting in the formation of "dihydride" residue. The former one can be utilized in hydrogen storage applications while the latter one can be used for hydrogen activation. When considering the interaction of single H_2 molecule with Sc-, Ti-, or V-decorated CC, the formation of dihydride residue is energetically favored over the formation of Kubas interaction. However, with increasing number of H_2 molecules, these two types of systems become almost equal in energy (energy difference being approximately 1 kJ mol^{-1}) [4]. It suggests that there is a dynamic co-existence of these two types of metal-hydrogen interaction which is further confirmed by ab initio molecular dynamics simulations. Regardless of type of interaction (Kubas or dihydride) the strength of formed bonds follows the order: Sc-H < Ti-H < V-H. Conversely, number of H_2 molecules interacting with metal-decorated CC follows the opposite trend: Sc-CC > Ti-CC > V-CC. For example, fully saturated Sc-decorated CC accommodates up to 16 H_2 molecules (see Figure 1) which corresponds to gravimetric density of 4.5 wt%.

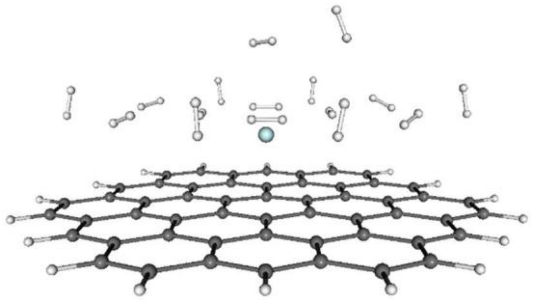


Figure 1: Optimized structure of Sc-decorated CC saturated with 16 H_2 molecules

Acknowledgements: This work received financial support from Slovak Grant Agencies APVV (contracts No. APVV-24-0207, APVV-23-0006, and VV-MVP-24-0039) and VEGA (contracts No. 1/0324/24 and 1/0175/23).

References:

[1] M. Malček, D.N. Sredojević, O. Tkáč, L. Bucinsky, Diam. Rel. Mat. 139 (2023) 110335.
[2] S. Mullerová, M. Malček, L. Bucinsky, M.N.D.S. Cordeiro, Carbon Lett. 34 (2024) 1495–1506.
[3] G.J. Kubas, J. Organomet. Chem. 635 (2001) 37–68.
[4] I.V. Voroshylova, O. Tkáč, L. Bucinsky, M. Malček, Int. J. Hydrogen Energy (2025) under revision

GAMMA IRRADIATION IMPACT ON MECHANICAL, STRUCTURAL AND OPTICAL PROPERTIES OF NATURAL LEATHER

Milica Maričić (0000-0002-9631-7779)[1], Mina Medić (0000-0001-8950-2426)[1], Jovana Periša (0000-0002-4683-0603)[1], Dušan Milivojević (0000-0001-8924-2679)[2], Miljana Popović (0000-0002-4691-0603)[3], Miroslav Dramićanin (0000-0003-4750-5359)[1]
[1]*Centre of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia*
[2]*Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, P.O. Box 522, 11000 Belgrade, Serbia*
[3]*Faculty of Technology and Metallurgy, University of Belgrade*
msekulic@vinca.rs

Gamma irradiation was investigated as a disinfection method for traditionally processed Balkan leathers, including calf, bovine, goat, and sheep. Samples were irradiated at doses of 0 (reference), 3, 5, 10, and 25 kGy using a cobalt-60 source, followed by long-term monitoring under museum-like conditions. To evaluate structural, chemical, and functional stability, a set of complementary techniques was applied: tensile testing for mechanical performance, Fourier-transform infrared spectroscopy (FTIR) for molecular changes, electron paramagnetic resonance (EPR) for radical species detection, and colorimetry (CIE Lab* and ΔE00) for chromatic stability. The collected data were processed with statistical analysis to assess whether the observed variations exceeded the experimental error range.
This comprehensive evaluation provides insight into the irradiation response of heritage leathers and supports the potential application of gamma irradiation as a conservation tool for the safe treatment of biologically vulnerable leather artifacts.

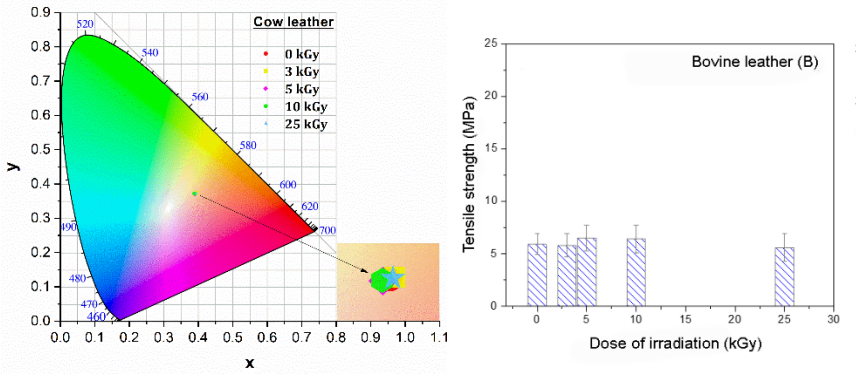


Figure 1. Bovine leather samples irradiated at different gamma doses: a) CIE chromaticity diagram; b) Tensile strength.

O-12

INDIRECT EPR STUDY OF TiO_2 MODIFIED WITH NATURAL EXTRACTS

Miriama Malček Šimunková (0000-0002-4035-4140)[a], Valentina Nikšić (0000-0003-2428-1225)[b] , Vesna Lazić (0000-0001-6440-6577)[b], Karol Lušpai (0000-0001-9653-7440)[a]

[a] *Institute of Physical Chemistry and Chemical Physics, Faculty of Chemical and Food Technology, Slovak University of Technology in Bratislava, Radlinského 9, SK-812 37 Bratislava, Slovak Republic, miriama.simunkova@stuba.sk*

[b] *Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade, Centre of Excellence for Photoconversion, P.O. Box 522, 11001, Belgrade, Serbia,*

This study investigates the photocatalytic behavior and radical-scavenging properties of titanium dioxide (TiO_2) functionalized with *Equisetum arvense* (horsetail) and *Camellia sinensis* (green tea) extracts. Natural polyphenols from the extract were incorporated into TiO_2 to form an interfacial charge transfer (ICT) complex, aiming to enhance visible-light responsiveness and manage radical scavenging properties through a green synthesis approach. Indirect electron paramagnetic resonance (EPR) techniques [1], including spin-trapping with DMPO, were applied to monitor photogenerated radical species. Results confirmed efficient production of ROS under UV-light excitation and the formation of hydroxyl and carbon-centered radicals, with reduced overall radical intensity compared to pristine TiO_2, indicating partial radical-scavenging by surface-bound organic moieties.

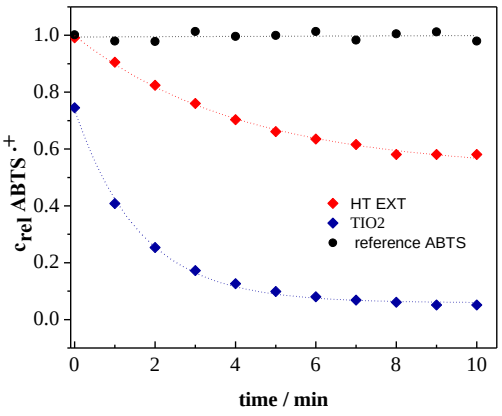


Figure 1. Time dependence of $ABTS^{\bullet+}$ relative concentration on time (LED@365 nm exposure, irradiance 20 mW cm^{-2}) evaluated from double-integrated EPR spectra monitored in the aqueous aerated suspensions of TiO_2 and TiO_2 /HT-EXT

Additional antioxidant capacity tests using DPPH and $ABTS^{\bullet+}$ assays [2, 3], revealed limited but detectable scavenging effects, suggesting that phenolic (–OH) groups are largely immobilized on TiO_2 surface, following the ICT complex formation. Further decrease in $ABTS^{\bullet+}$ EPR signal intensity was found under UV-light (LED@365nm) excitation (Fig. 1).

The findings highlight that TiO_2 modified with natural extract as a promising hybrid photocatalyst with combined charge carrier generation and moderate radical-scavenging potential.

Acknowledgements: This work was supported by the Research and Development Support Agency project under contract no. VV-MVP-24-0039 *and bilateral project SK-SRB-23-0021*.

[1] V. Nikšić et al. *Optical Materials* 152 (2024) 115454.
[2] M. Štekláč et al *Journal of Inorganic Biochemistry* 264 (2025) 112802.
[3] A. Staško et al. *Free Radical Research* 41 (2007) p. 379-390.

O-13

RAPID SYNTHESIS OF YBO_3 AS HOST MATERIALS FOR Pr^{3+} DOPING

Radu Banica (0000-0002-9435-2837)[a], Vlad Socoliuc (0000-0003-0529-1911)[b], Poienar Maria (0000-0002-0841-3286)[c], Rus Stefania (0000-0001-8505-0733)[a], Casut Cristian[a], Cristina Mosoarca (0000-0001-9969-4900)[a], Zeljka Antic (0000-0002-7990-2001)[a,d], Miroslav Dramicanin (0000-0003-4750-5359)[a,d]

[a]*National Institute of Research and Development for Electrochemistry and Condensed Matter, Str. Dr. A. Păunescu Podeanu nr.144, 300569 Timisoara, Romania; radu.banica@yahoo.com;*

[b]*Romanian Academy-Timisoara Branch, Center for Fundamental and Advanced Technical Research, Lab. Magnetic Fluids, 24 M. Viteazu Ave., RO-300223 Timisoara, Romania;*

[c]*Institute for Advanced Environmental Research, West University of Timisoara (ICAM-WUT), Oituz Str., No. 4, 300086 Timisoara, Romania;*

[d]*Centre of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences—National Institute of the Republic of Serbia, University of Belgrade, Mike Petrovića Alasa 12-14, 11000 Belgrade, Serbia.*

The spread of antibiotic-resistant bacteria over the last decade demands the development of new materials and techniques for disinfection of water and surfaces. Because natural sunlight at ground level contains only low levels of UVC radiation, most bacteria have not developed resistance to this spectral band, and UVC remains an effective means for surface disinfection in hospitals as well as for biological treatment in some drinking-water facilities. Materials capable of efficient photonic up-conversion to the UVC range therefore represent a promising, low-cost strategy to convert sunlight into germicidal radiation. Additionally, several yttrium-based compounds exhibit direct bactericidal activity, either through ion release (e.g. Y^{3+}) or via interactions between microbial cell walls and crystal surfaces.

In this work we focus on the synthesis and characterization of YBO_3 as a host material for subsequent Pr^{3+} doping, combining the potential for up-conversion emission in the germicidal region with possible non-radiative bactericidal effects. YBO_3 was prepared by a solid-state route using two different yttrium precursors: (i) a commercial yttrium oxide and (ii) Y_2O_3 nanoparticles produced at low temperature in polyol media. Both precursors and the resulting YBO_3 products were characterized by X-ray diffraction, scanning electron microscopy, Fourier transform infrared spectroscopy, UV–Vis–NIR spectrophotometry, dynamic light scattering and thermogravimetric analysis.

We observe a decisive influence of the yttrium precursor on reaction kinetics and required thermal budget. Using the polyol-derived Y_2O_3 nanoparticles, the pure ternary YBO_3 phase forms at only 800°C with reaction times below 10 minutes. By contrast, the commercial precursor yields residual unreacted Y_2O_3 even at reaction times more than three times longer and at temperatures 100 °C higher. The rapid route therefore lowers the calcination energy demand and produces YBO_3 particles with smaller dimensions than those obtained through conventional high-temperature, long-duration syntheses.

Acknowledgements: This study was supported by Romania's National Recovery and Resilience Plan, PNRR [project grant number C9-I8-28/FC 760107/2023].

O-14

PHYSICS-INFORMED ARTIFICIAL INTELLEGENCE FRAMEWORK FOR PREDICTING LUMINESCENCE PROPERTIES OF Cr^{3+}-DOPED INORGANIC PHOSPHORS

Snežana Đurković (0009-0007-6638-0682), Zoran Ristić (0000-0002-1854-284X), Miroslav Dramićanin (0000-0003-4750-5359)
Centre of Excellence for Photoconversion, Vinča Insitute of Nuclear Sciences—National Institute of the Republic of Serbia, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia
snezana.djurkovic@vin.bg.ac.rs, risticz@vin.bg.ac.rs, dramican@gmail.com

We present a cutting-edge physics-informed artificial intelligence (AI) approach for accelerated discovery of Cr^{3+}-doped inorganic phosphor materials with tailored luminescence properties. Our approach integrates fundamental crystal field theory principles with advanced machine learning (ML) algorithms to efficiently identify promising candidates for solid-state lighting, optical sensors, and bio-imaging applications. We develop a systematic data-driven methodology to capture complex nonlinear relationships between structural and optical characteristics in Cr^{3+} -doped oxide host materials. Our comprehensive dataset combines information from peer-reviewed literature for crystal field data and respectable crystallographic databases (Materials Project and Crystallography Open Database) for structural ones, focusing on single and double-layered perovskites with octahedral Cr^{3+} substitution sites. Key structural descriptors include bond lengths, angular distortions of octahedra, and other coordination environment parameters extracted using VESTA software. Optical properties are characterized using Tanabe-Sugano diagram as indispensable theoretical foundation for obtaining important crystal field parameters from photoluminescent spectra, correlating crystal field strength ratios (Dq/B) with electronic energy levels ^2E_g, $^4T_{2g}$, and $^4T_{1g}$ of d^3 electron systems [1]. A well-defined feature engineering process ensures a reliable, high-quality initial dataset for further pattern recognition between structural and optical parameters. The computational framework employs two complementary ML approaches [2], including model training and validation-interpretable “white-box” random forest (RF) algorithms providing transparent feature importance analysis, and “black-box” artificial neural networks (ANN) for capturing complex nonlinear relationships with hyperparameter optimization. The framework is designed to identify high-performance candidates that can be subsequently validated through experimental synthesis and characterization. This methodology represents a significant advancement in computational materials discovery for luminescent materials, offering a systematic pathway for next-generation red phosphor discovery and development.

References

[1] Sadao Adachi, Review—Photoluminescence Properties of Cr3+-Activated Oxide Phosphors, *ECS J. Solid State Sci. Technol.* 10 (2021) 026001.
[2] Suresh R, Bishnoi H, Kuklin AV, Parikh A, Molokeev M, Harinarayanan R, Gharat S and Hiba P, Revolutionizing physics: a comprehensive survey of machine learning applications. Front. Phys. 12 (2024), 1322162.

O-15

Cr^{3+} DOPED CALCIUM STANNATE PERSISTENT LUMINESCENCE MATERIAL

Sofia Maleeva[a] (0009-0008-2832-0811), Maxim Ivanov[a] (0000-0003-2777-8421), Zoran Ristić[a] (0000-0002-1854-284X), Miroslav D. Dramićanin[a] (0000-0003-4750-5359)
[a]*Centre of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences -National Institute of the Republic of Serbia, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia,* maleevsof@gmail.com

Chromium-doped (Cr^{3+}) phosphors are the subject of intensive research encompassing key fields such as optoelectronics, materials science, and biomedicine [1,2]. Cr^{3+} ions, acting as efficient activators, enable broadband near-infrared (NIR) emission with tunable wavelength and spectral distribution, which is critical for creating high-performance optical systems [3]. The practical application of these materials spans a wide range of high-tech domains, including bio-imaging, where NIR emission provides deep penetration into biological tissues and high contrast [4], and the development of miniature spectrometers based on phosphor-converted light-emitting diode (pc-LED) technology [2]. In this work, calcium stannate ($CaSnO_3$) is investigated as an intermediate crystal field oxide host for Cr^{3+} ions. Co-doping with gadolinium was used to stabilize oxidation state of Cr^{3+} and modify crystal field of the matrix. $CaSnO_3$:Cr^{3+},Gd^{3+} powders were synthesized by a solid-state reaction at the temperature of 1400°C. X-ray diffraction (XRD) confirmed the successful formation of an orthorhombic $CaSnO_3$ phase. Scanning electron microscopy (SEM) was used to characterize the powder morphology. The powder was found to have a bimodal particle size distribution, comprising two distinct morphological fractions: primary particles and their agglomerates. The size difference between the primary particles (1.5–2 μm) and agglomerates (15–25 μm) is approximately one order of magnitude, providing a basis for efficient fraction separation via sedimentation. Luminescent properties of the material were investigated in detail and concentration of the dopants was optimized. An intense broadband luminescence of Cr^{3+} ions in the NIR range (700-900 nm) was observed. Furthermore, the material was found to exhibit persistent afterglow, which is of interest for applications requiring prolonged emission. The results confirm that $CaSnO_3$:Cr^{3+},Gd^{3+} is a promising phosphor for near-infrared light generation, featuring the beneficial property of persistent luminescence.

References:
[1] Fang, Mu-Huai, et al. "Penetrating biological tissue using light-emitting diodes with a highly efficient near-infrared ScBO3: Cr3+ phosphor." *Chemistry of Materials* 32.5 (2020): 2166-2171.
[2] Rajendran, Veeramani, Ho Chang, and Ru-Shi Liu. "Recent progress on broadband near-infrared phosphors-converted light emitting diodes for future miniature spectrometers." *Optical Materials: X* 1 (2019): 100011.
[3] Zhao, Fangyi, Zhen Song, and Quanlin Liu. "Advances in chromium-activated phosphors for near-infrared light sources." *Laser & Photonics Reviews* 16.11 (2022): 2200380.
[4] Marcos-Vidal, A., J. J. Vaquero, and J. Ripoll. "Near Infrared-Emitting Nanoparticles for Biomedical Applications." (2020): 1-20.

O-16

UP-CONVERSION LUMINESCENCE AND LIFETIME THERMOMETRY IN Er^{3+}/Yb^{3+}-DOPED $YNbO_4$ NANOPHOSPHORS

Tamara B. Ivetić (0000-0001-8353-9033)[a], Ljubica Đačanin Far(0000-0002-0760-3758)[b], Zoran Ristić(0000-0002-1854-284X)[b]

[a]*University of Novi Sad, Faculty of Sciences, Department of Physics, Trg Dositeja Obradovića 3, 21000 Novi Sad, Serbia, tamara.ivetic@df.uns.ac.rs*

[b]*Center of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade, 11001 Belgrade, Serbia, ljubica.far@vin.bg.ac.rs, zoran.s.ristic@gmail.com*

Rare-earth-doped niobates have emerged as robust candidates for optical thermometry owing to their chemical stability and efficient up-conversion (UC) luminescence [1,2]. In this work, we present Er^{3+}/Yb^{3+} co-doped $YNbO_4$ nanophosphors synthesized via a mechanically activated solid-state route [3]. Structural and morphological analyses confirmed the formation of a monoclinic fergusonite phase composed of nanocrystalline domains with micrometer-sized agglomerates. Elemental mapping revealed uniform dopant distribution throughout the grains. Under 980 nm excitation, the phosphors exhibited intense green and red UC emissions corresponding to Er^{3+} transitions sensitized by Yb^{3+} ions [4,5]. The dominant green band ($^4S_{3/2} \rightarrow {}^4I_{15/2}$) exhibited a lifetime of 238 μs at room temperature. Temperature-dependent lifetime studies (300–600 K) showed systematic quenching behavior, yielding a maximum relative sensitivity of 2.3×10^{-3} K^{-1} near 300 K [6,7]. These findings confirm $YNbO_4$:Er,Yb as a stable oxide-based platform for reliable lifetime thermometry, particularly suitable for harsh or chemically demanding environments where durability is essential.

Acknowledgements: This work was financed by the APV Provincial Secretariat for Higher Education and Scientific Research (Project title: "Development of new highly-sensitive sensors for monitoring of gas pollution and humidity in Vojvodina" contract no. 003075795 2024 09418 003 000 000 001/2). The authors also gratefully acknowledge the financial support of the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Grants No. 451-03-137/2025-03/ 200125 & 451-03-136/2025-03/ 200125).

Reference to a journal publication:

[1] X. Wang, X. Li, H. Zhong, S. Xu, L. Cheng, J. Sun, J. Zhang, L. Li, B. Chen, Sci. Reports 8 (2018) 5736.
[2] Lj.R. Đačanin, M.D. Dramićanin, S.R. Lukić-Petrović, D.M. Petrović, M.G. Nikolić, Cent. Eur. J. Phys. 10 (2012) 519–523.
[3] Lj.R. Đačanin, M.D. Dramićanin, S.R. Lukić-Petrović, D.M. Petrović, M.G. Nikolić, T.B. Ivetić, I.O. Gúth, Ceram. Int. 40 (2014) 8281–8286.
[4] C.K. Lee, Y.J. Kim, Ceram. Int. 48 (2022) 3985–3992.
[5] X. Wang, X.P. Li, Y. Zhang, B. Chen, J. Luminescence 263 (2023) 120055.
[6] Y. Tian, Y. Tian, P. Huang, L. Wang, Q. Shi, C. Cui, Chem. Eng. J. 297 (2016) 26–34.
[7] Z. Ristić, W. Piotrowski, M. Medić, J. Periša, Ž.M. Antić, L. Marciniak, M.D. Dramićanin, ACS Appl. Electron. Mater. 4 (2022) 1057–1062.

O-17

THE ION-DOPING OF MESOPOROUS BIOACTIVE GLASS PARTICLES

Tamara Matic[a] (0000-0002-7415-0453), Teodora Jakovljevic[b], Vukasin Ugrinovic[b] (0000-0002-5809-8712), Nemanja Barac[b] (0000-0001-5037-9176), Djordje Janackovic[a] (0000-0002-8291-4345), Rada Petrovic[a] (0000-0001-9511-5633), Djordje Veljovic[a] (0000-0001-6370-7167)

[a]*University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia*
[b]*Innovation Center of the Faculty of Technology and Metallurgy Ltd, Belgrade, Serbia*

Mesoporous silica has been extensively studied over the past 25 years, mainly for application in biomedicine, drug delivery, catalysis, adsorption, and energy storage, owing to its high specific surface area and mesoporous channels. The introduction of Ca^{2+} ions into the silica network led to the development of mesoporous bioactive glass particles (MBGs) – representing the latest generation of bioactive glasses. Further incorporation of therapeutical elements such as Sr, Mg, Zn, Ag, Se, allows stimulation of a specific biological response, including enhanced bone regeneration, immunomodulation, antimicrobial or antitumor activity, while maintaining the capacity to carry drugs and growth factors. As a results, ion-doped MBGs are among the most actively investigated materials for biomedical application, including wound healing, bone and tendon regeneration, dental application, drug delivery, biosensing, and theranostics.
Ion-doping, and specifically multi-ion-doping, can alter MBGs mesostructure, influencing dissolution behavior, drug loading capacity and drug release profile. Here, we present the effects of synthesis parameters and composition on the MBG structure and drug delivery properties. Furthermore, we investigate the influence of binary ion-doping with Sr^{2+} and Mg^{2+} ions, as well as multi-ion doping with Sr^{2+}, Mg^{2+}, Cu^{2+}, Zn^{2+} ions, on the *in vitro* biocompatibility, pro-osteogenic and pro-angiogenic properties, as well as antimicrobial activity. Our results demonstrate that careful optimization of synthesis conditions and composition is essential to tailor MBG properties for specific application.

Acknowledgements: This research was funded by the Science Fund of Republic of Serbia #GRANT No.7470, *Novel hybrid biomimetic macroporous composites with tuned biodegradability, improved osteointegration and anticancer properties for bone tissue regeneration* – HyBioComBone and by Ministry of Science, Technological Development and Innovations, Republic of Serbia (No. 451-03-136/2025-03/200135, 451-03-136/2025-03/200287)

O-18

ECO-SAFE BIOACTIVE TiO_2 NANOHYBRIDS FUNCTIONALIZED WITH GREEN TEA PHENOLICS

Valentina Nikšić (0000-0003-2428-1225)[a], Miljana Dukić (0000-0002-1556-0380)[a], Katarina Isaković (0009-0007-7150-706X)[a], Ana Milivojević (0000-0002-4894-9907)[b], Andrea Pirković (0000-0002-1182-4895)[c], Dušan Sredojević (0000-0003-2867-2047)[a], Vesna Lazić (0000-0001-6440-6577)[a]

[a] *Centre of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia* valentina.niksic@vin.bg.ac.rs
[b] *Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia*
[c] *INEP Institute for Application of Nuclear Energy, University of Belgrade, Belgrade, Serbia*

This study represents an approach for improvement of the optical properties of wide bandgap metal oxide – TiO_2, which is based on the formation of the inorganic-organic hybrids that display absorption in the visible spectral range due to the formation of interfacial charge transfer (ICT) complexes. The surface modification of TiO_2 was performed using green tea extract enriched with bioactive phenolic compounds. Additionally, we modified the nanocomposite through silver impregnation, resulting in an eco-safe nanohybrid with enhanced antimicrobial properties.

Characterization of TiO_2/GT/Ag nanohybrid was performed using spectroscopic and microscopic techniques. FTIR, XRD, and TEM analyses confirmed the successful synthesis of the nanohybrid. Compared to pristine TiO_2, DRS revealed a red-shifted absorption, indicating enhanced optical properties of the new nanomaterial.

Microbiological assays demonstrated that the synthesized nanohybrids achieve significantly enhanced antimicrobial activity against *E. coli*, *S. aureus*, and *C. albicans*, even at lower, non-toxic concentrations. Cytotoxicity tests conducted at the same concentrations on MRC-5 and HeLa cell lines confirmed high biocompatibility, with cell viability remaining above 75% even at the highest concentration tested. These findings highlight the nanohybrid's potential as a safe and effective alternative antimicrobial agent for wastewater treatment, where reduced cytotoxicity combined with high antimicrobial performance is critical.