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No. 20/2024

The International Symposium "Priorities of chemistry for a sustainable development"

PRIOCHEM

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under the aegis and with the support of the
Romanian Ministry of Research, Innovation and Digitalization

Partners: Romanian Chemical Society,
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FOREWORD

In a world of change, the National Institute for Research & Development in Chemistry and Petrochemistry ICECHIM Bucharest wants to adapt to the current reality, by combining tradition with the new. The International Symposium "Priorities of chemistry for a sustainable development" PRIOCHEM is the best example in this context, especially at its 20th edition.

2024 is an important year, as it marks not only this anniversary edition, but also ICECHIM's 20th anniversary as a national R&D institute. The institute was honored by the presence of representatives from the Ministry of Research, Innovation and Digitalization, the Romanian Chemical Society, the Romanian Chemical Engineering Society, the Romanian Academy, national R&D institutes, universities, as well as economic agents, media partners, special guests and participants from the international scientific community.

The impressive number of participants at the International Symposium PRIOCHEM is based on the institute's notoriety, the outstanding results achieved in recent years and the pleasant atmosphere that people are welcomed with every year.

Because PRIOCHEM 2024 deserved to be celebrated in the right way, a new concept was introduced this year: “Tech Talks - Meet the Mentors!”. The idea came from the desire to help students and young researchers engage with distinguished researchers from various scientific and technological fields, representing today’s and tomorrow’s mentors across several areas of expertise. Also, the early-stage researchers could discover prevailing and emerging scientific areas of intense interest and research focus.

ICECHIM has encouraged networking since always, so the participants were glad to join in the discussions about science, career and personal experiences in R&D.

The 20th anniversary edition of PRIOCHEM was organized under the aegis and with the support of the Romanian Ministry of Research, Innovation and Digitalization, in partnership with the Romanian Chemical Society and the “C.D. Nenițescu” Foundation. At the same time, the event was a great success thanks to the sponsors Brenntag, NanoTeam, MDPI and Avantor.

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Porous materials and molecularly imprinted polymers for removal and quantification of organic contaminants

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Keywords: molecularly imprinted polymers, porous adsorbents, quantification, organic contaminants

Introduction: Porous polymers and molecularly imprinted polymers (MIPs) have emerged as versatile materials for the selective removal and detection of organic contaminants in environmental and biological systems. Their high surface area, tunable porosity, and tailored molecular recognition sites enable the efficient capture of various pollutants, including pesticides and parabens, which are of significant concern due to their persistence and potential health risks.

Materials and methods: Our work focuses on the synthesis of porous polymers and MIPs designed for the selective adsorption of these contaminants [1,2]. By optimizing the polymerization conditions, including the choice of starting polymers and monomers, crosslinkers, and imprinting molecules, we successfully developed materials with enhanced binding affinities and selectivities. These polymers offer significant improvements over traditional sorbents, exhibiting higher capacities and faster adsorption kinetics.

In addition to the synthesis, we present a novel application of these materials in conjunction with ambient mass spectrometry (AMS). AMS, with its ability to analyze samples in their native state without extensive sample preparation, provides a powerful tool for the rapid and direct quantification of contaminants adsorbed onto the polymer surfaces. Our integrated system allows for real-time monitoring of adsorbed analytes, enabling quantification directly from the polymer surface without the need for elution or derivatization. This approach enhances both the speed and accuracy of contaminant detection, while also minimizing the consumption of solvents and reagents [3, 4].

Results: We demonstrate the utility of this method through the detection and quantification of pesticides and parabens from water samples. The high sensitivity and specificity of the MIP-AMS system make it a promising platform for environmental monitoring and contamination control. Moreover, the flexibility of this approach allows for the potential expansion to other organic pollutants, making it a highly adaptable tool in analytical chemistry.

In summary, our work highlights the potential of porous polymers and MIPs not only as efficient adsorbents but also as integral components in a direct, real-time analytical platform for organic contaminant quantification. This interdisciplinary approach combines material science with cutting-edge analytical techniques, offering a sustainable and efficient solution for environmental monitoring.

***Acknowledgements**: This work was supported by the National Science Centre, Poland, under grant number 2020/37/B/ST5/01938.*

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FLUIDIC ELECTROCHEMICAL DEVICES ON PAPER WITH INTEGRATED FLEXIBLE ELECTRODES

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Keywords: electrospinning, flexible, electrodes, paper, microfluidics, point-of-care

Introduction: Flexible porous materials have gained a high interest due to their impact on the development of electrochemical point-of care (PoC) devices for monitoring the state of health of individuals. Among the porous materials, paper is the most commonly used due to its innate capillary action on fluids. The patterning of hydrophilic and hydrophobic regions for sample flow control is considered. On another hand, electro spun polymeric fibers (EPF) present an emerging alternative for the development of flexible electronics, enabling applications in PoC testing devices. The integration of chromatographic paper with EPF is described.

Materials and methods: The development of the paper-based electrochemical cell consists of three main steps: *i)* electrodes fabrication by electrospinning and their metallization; *ii)* chromatographic paper patterning with channels and test zones; and *iii)* assembling the electrodes with the paper.

Results: This work presents a novel approach to obtain fluidic electrochemical devices that integrate flexible electrodes directly onto paper substrates using EPFs, ***Figure* 1**. These fibers are metallized to form conductive networks, enabling enhanced electrochemical performance while maintaining the inherent flexibility. The use of electrospinning allows for precise control over the fiber morphology and the incorporation of active materials, making these devices adaptable for a wide range of sensing and analytical applications. Among these, wearable sensors and biosensors for detection of some biomarkers such as ions (H^+, Ca^{2+}, Na^+, NH_4^+, Cl^-), glucose and uric acid in sweat at epidermal level, or in other body fluids, are described. Another application is related to the quantification of nucleic acids from different origins and their *in-situ* amplification by polymerase chain reaction (PCR). The development of microheaters capable to perform accurate thermal cycles essentials for nucleic acids amplification by PCR is discussed.

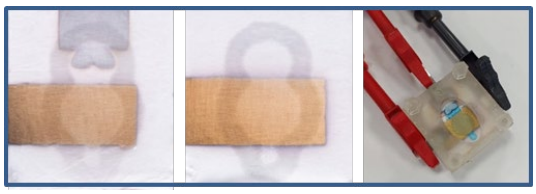

***Figure 1**. Photographs of a microfluidic electrochemical cell obtained by integrating EPF electrodes with chromatographic paper.*

Conclusions: The results demonstrate the effective integration of these polymeric fibre-based electrodes into paper-based microfluidic channels, providing a robust platform for real-time electrochemical sensing. This innovation offers significant potential for applications in healthcare diagnostics, and point-of-care testing.

***Acknowledgements**: Financial support from the Executive Agency for Higher Education and Research Funding (UEFISCDI) through project PN-III-P4-PCE-2021-1006.*

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A concrete case of rheology use as a powerful research method in chemical engineering and medical sciences

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Keywords: rheology, nonnewtonian fluids, gelatine hydrolysis, triferment, starch, hydrolysis

Introduction: The monitoring of rheological properties, by establishing the correlation between viscosity and shear rate, regards an important tool in food and drug industry during the development of semisolid dosage forms since it sheds light on why some formulations flow, while others retain structure under shear [1]. Fluids or food or drug formulations that deform after exceeding a threshold value of the deformation effort are fluids of the real plastic type, respectively Bingham [2]. An important number of models to express the relationship between the shear stress and the shear rate have been proposed. These models are recognized as fluid rheological state equations. These can define almost all fluids except those with viscoelastic behavior [2]. Viscous fluid models characterize such type fluid by identifying the participation of the viscous and elastic parts in it, as well as their coupling mode of the two parts. When the viscosity of a fluid evolves over time, it shows that a chemical or biochemical process is taking place inside it. Such a situation happens with food fluids when enzymes arrive in them that cause hydrolysis reactions of its components. In cases of pancreatic insufficiency, the supplementing with digestive enzymes, for hydrolysis of food, is supported by specific drugs [3], as in the case of Triferment and Colebil.

Materials and methods: The present work proposes the in vitro hydrolysis of gelatine protein and starch media in the presence of Triferment drug. The method for highlighting hydrolysis consists in registration of time dynamics of apparent viscosity of the gelatin or starch solutions, in which Triferment was dosed. With respect to concentration of the hydrolysable species, the pH and the temperature of the hydrolysis medium it shows that they were fixed to reproduce the digestion conditions of. The part of the mathematical modeling related to the experimental investigation is focused on the determination of the kinetic parameters, which characterize the hydrolysis with Triferment of specific gelatin or starch media. In this sense, to create a relation between medium viscosity and medium composition admits that both the concentration of biopolymer in the medium and the degree of polymerization, linearly depend on the biopolymer conversion (the conversion of gelatin respectively of starch into amino acids constituents respectively sugars).

Results: The finding that Triferment tablets over 1 year old lose a lot of their ability to hydrolyze gelatin solutions is quantitatively expressed by comparing the values of the constants of the hydrolysis model for comparing casses.

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AEROGELS PRODUCTION FROM PET WASTES

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Keywords: aerogel, circular economy, wastes, PET

Introduction: Plastic bottles are mostly single-use plastics that, when incorrectly discarded in the environment originate microplastics, with serious effects in the ecosystems. Therefore, the development of new value-added products with longer service life, through chemical reprocessing, can contribute to the creation of new cycles with extended raw materials profitability in the products chain.
On the other hand, aerogels are recognized by their unique thermal superinsulation performance. Their extensive mesoporous network, with porosities often surpassing 90%, leads to high-efficiency in the heat transfer blocking due to the Knudsen effect [1,2]. Other surface and porosity related properties, as very low bulk densities (30-300 kg/m^3) and extremely high BET surface area (300-1000 m^2/g) are strongly appreciated for other applications such as sorption, catalysis, encapsulation or controlled release of active substances. However, the production cost of aerogels remains high, mainly due to the need for expensive precursors and long diffusion-driven solvent exchanges. Also, their environmental footprint can be lowered if a more circular approach is integrated in the synthesis process.
In this work, recycled poly(ethylene terephthalate) (rPET) aerogels entirely obtained from plastic bottles were obtained with thermal conductivities comparable to commercial thermal insulators.
Materials and methods: Drinking water bottles were cut to obtain small pieces of rPET, which were dissolved and then transformed into a gel through the addition of a non-solvent. The gel was washed with water and freeze-dried to originate the aerogel. Unreinforced and fiber-reinforced aerogels (with silica or PET fibers) were prepared by this method.
Results: The aerogel products had bulk densities as low as 150 kg/m^3, porosities above 80% and elasticity modulus in the order of units of MPa. Their thermal conductivity was in the range ~30-50 mW/m.K. The followed circular approach contributes to the achievement of EU energy efficiency directives and climate action targets in the medium term.

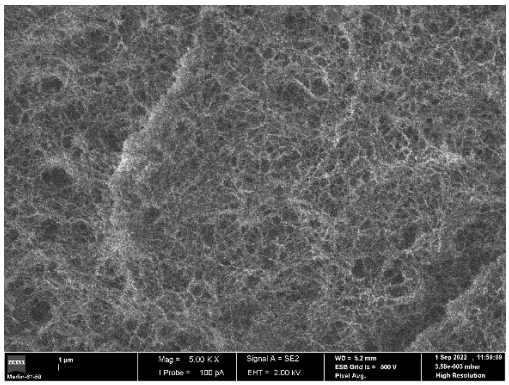

Figure 1. Unreinfoorced rPET aerogels porous nanostructure.

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POLITEHNICA Bucharest: Teaching and R&D Capabilities in Tissue Engineering

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National University of Science and Technology POLITEHNICA Bucharest (POLITEHNICA Bucharest) is one of the oldest technical university from the Romania which, upon the absorption of the University Pitesti, became one of the largest comprehensive university from Romania. Considering the over 205 years of excellence in the fields of engineering and especially in the field of chemical engineering, we are focusing our efforts in developing new materials and technologies for the society, including for Health.

In the last period of time, our team was mainly involved in developing new materials or to modify them according to different chemical routes. In the last decade, the mostly studied materials for tissue engineering were: composite materials for bone regeneration and derived drug delivery systems for the treatment of different bone-related diseases (including a large variety of 3D printed scaffolds for specific applications); 2D materials especially graphene oxide including electrospun mats; 1D nano- and microfibers (especially by electrospinning) or 0D materials (AgNPs, Fe_3O_4, ZnO, hydroxyapatite etc.) for soft tissue engineering. Along with these, a special attention was devoted to the surface modification of different medical devices (catheters, stents, wound dressings etc.) or protective devices (especially for anti-adherent and antimicrobial activity).

In all these researches, teaching component is very important because a major role is belonging to the students (including MSc and PhD students) and postdocs which are getting skills and knowledge in designing and developing such materials for specific applications.

Acknowledgments: *The authors are acknowledging the support of the project ERANET-FLAG-ERA-Smart2Graph-1: "Smart nerve grafts based on graphene-related composite materials with electric-triggering capability for central and peripheral nervous system regeneration" and "Grefe osoase nanostructurate cu proprietăți prestabilite" - PN-IV-P8-8.3-ROMD-2023-0347, contract no. 29ROMD, 20/05/2024.*

TiO_2-based nanomaterials with single-atom co-catalysts in photocatalysis

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Keywords: TiO_2 nanotubes, co-catalysts, single-atom, H_2 production

Introduction: Green hydrogen production based on TiO_2-based materials means overcoming TiO_2's limitations, which are slow kinetics and no visible range response. To reach reasonable photocatalytic reaction rates, noble metals, such as Pt, Pd, Rh, Au, etc., are used as co-catalysts on the surface of the semiconductor, either in the form of metallic nanoparticles (NPs) or, more recently, as single-atom (SA). Combining high-aspect ratio TiO_2 nanotubes [1] with SA results in a significant enhancement in the photocatalytic H_2 production with a use of minimal noble metal amount [2–4].

Materials and methods: TiO_2 nanotubes were obtained by electrochemical anodization of Ti and annealed to anatase [3]. The single-atom decoration of Pt, Pd, Rh, and Au onto the TiO_2 was achieved through reactive deposition in a noble metal precursor solution, as described in our recent work [3]. Additionally, TiO_2 anodic nanotubes layers can be decorated by CdS, and further decorated with Pt SA [4]. For more details on the used characterization techniques (SEM, XPS, TEM) and H_2 photocatalytic measurements, see reference [3,4].

Results: The present study examines recent advancements in the single-atom (SA) co-catalyst decoration of anodic TiO_2 nanotubular layers and the application of such SA-decorated NTs in photocatalytic H_2 production. This research demonstrates that anodic TiO_2 nanotubes can serve as a substrate for the decoration with noble metal single atoms, SAs, including Pt, Pd, Rh, and Au, through a straightforward "reactive deposition" method. Furthermore, these SA-decorated TiO_2 NTs exhibit enhanced activity for photocatalytic H_2 generation from pure water, without the presence of a sacrificial agent, in comparison to their nanoparticle counterpart decorated tube layers. As an additional example, in the case of a hierarchical structure based on CdS-decorated TiO_2 nanotubes, where decoration with Pt SAs, which bind to both the TiO_2 and CdS, results in increased photocatalytic H_2 production.

Conclusions: This study summarizes TiO_2 NTs produced through electrochemical anodization and their single-atom co-catalyst decoration via reactive deposition, comparing the photocatalytic H_2 generation efficiency of TiO_2 NTs decorated with various noble metal SAs (Pt, Pd, Rh, Au) against their nanoparticle counterparts. The results indicate a significant advantage of using SAs for efficient H_2 production from plain water. Additionally, the Pt SA binding on hierarchical substrates (CdS-TiO_2 nanotubes) demonstrates the observable Pt SA binding on different supports.

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Effect of nanofillers in the ageing of polymer matrix composites (PMCs)

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Keywords: polymer matrix composites, nanofillers, photo-oxidative aging, hydrothermal aging

The incorporation of nano-objects (carbon nanotubes, graphene, silica, lamellar fillers etc.) into polymer matrices for mechanical reinforcement has been widely studied. One of the main difficulties encountered with this type of material lies in achieving a fine, homogeneous dispersion of the nano-objects within the polymer matrix.
The high specific surface area of nano-objects considerably increases their tendency to self-aggregate. One way of improving dispersion is to chemically modify nano-objects to improve their compatibility with the polymer matrix.
These chemical treatments can modify the behavior of the material with respect to environmental constraints such as hydrothermal stresses. Also, certain types of nano-objects are not chemically inert to external stresses, and that these evolutions must be taken into account in the evolution of the material's macroscopic properties.

Development, Application, and Evaluation of ORMOCER®- Based Protective Coatings for Cultural Heritage Preservation

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ORMOCER®s (organically modified ceramics) are hybrid polymers that combine inorganic and organic structures through the hydrolysis and condensation of silicon and metal alkoxides, as well as organo(alkoxy)silanes.

The sol-gel-like process generates colloidal solutions that form low-molecular oligomers, which can subsequently be processed into high-molecular weight products. The material properties can be precisely tailored to meet contemporary conservation standards by selecting suitably functionalized starting materials. In contrast, conventional polymer-based materials are not designed for the long-term preservation of cultural heritage objects, often suffering from inadequate adhesive strength, suboptimal elasticity, and poor aging characteristics, including chemical degradation, discoloration (mainly yellowing), and limited reversibility.

Over 30 years ago ORMOCER®s were applied to significant cultural monuments, such as the Cologne Cathedral and have been re-evaluated in 2021 using vibrational spectroscopy. The examination revealed that the material remained fully intact even after three decades of outdoor exposure, underscoring its excellent long-term durability and potential as a reliable solution for the conservation of cultural heritage.

NOVEL CARBON NANOMATERIALS – COMPARISON OF GRAPHENE, CARBON FOAM AND GRAPHITE

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Keywords: carbon nanomaterials, XRD, Raman spectroscopy

Introduction: Important group of composite materials is polymer carbon composites composed of a polymer matrix and various forms of carbon; carbon fibers, carbon black, and graphite, have been widely used as fillers for a large spectrum of polymers. Recently, carbon nanomaterials, i.e. nanofibers, nanotubes, graphene materials, and other forms of nanocarbons, have received widespread interest.
Carbon foam is advanced nanoporous material with multiple high-technology applications, due to its cell structure, light weight, high thermal stability, high thermal and electrical conductivity, as well as exceptional electromagnetic and acoustic properties. Graphene has become a valuable and useful nanomaterial due to its exceptionally high tensile strength, electrical conductivity, transparency, and being the thinnest two-dimensional material in the world. Carbon materials with a variety of pore and particle size, morphology and volume, can be synthesized, using different precursors and methods. Carbon foam have different possible high-technology applications, due to its unique characteristics - cell structure, light weight, high thermal stability, high thermal and electrical conductivity, electromagnetic, irradiation and acoustic properties, etc. In addition, carbon foams have been tested for use as a thermal energy storage container and material enhancing thermal conductivity, for various electrochemical measurements as electrodes, for adsorption and desorption of gaseous species, for clean-up and recovery of spilled oils and other pollutants, and for reflection of electromagnetic waves. Carbon foam properties depend on cell structure, as well as on the structure and nanotexture of macropore walls. This gives possibilities for control of bulk properties during foaming process, in comparison to other carbon materials. The effect of the precursor on the structure and properties of obtained carbon foams is essential, so this issue is under extensive investigations. The development of carbon foams on the base of coal tar pitch provides an efficient way for production of light-weight strong carbon material. Usually, the commercial coal tar pitches need pretreatment before use, because their plastic properties (viscosity) do not meet the foaming requirements. Thermochemical treatment, air blow, and other oxidation procedures are well-known pretreatments for modifying the pitch characteristics, which in turn influences the foaming properties of the pitch precursor. The aim of the present investigation is to find precursors with appropriate composition, which together with precisely selected thermochemical modification of the precursors, to permit direct formation of "green" foam without pressure and without stabilization step. The main task is to find optimal composition of the precursor and treatment conditions, which allow synthesis of carbon foam with good mechanical strength and relatively regular pore structure. The formation mechanism of the porous structure of carbon foams is considered. Obtained samples (carbon foam, graphene, graphite) are characterized by XRD, Scanning Electron Microscopy, TG and DSC analysis, elemental analysis, mechanical strength. The proposed new, less energy consuming synthesis method enables the production of carbon foam with very good physico-chemical properties. Other aim of this work was to investigate the effect of the particle size distribution of carbon foams used as particulate fillers on the properties of their epoxy composites.
Materials and methods: The carbon foam polymer precursor was obtained by cross-linking of a low-molecular epoxy resin with phenol-formaldehyde resin. The epoxy resin Epidian 6 (supplied by Ciech Sarzyna S.A., Poland) is prepolymer of the diglycidyl ether of bisphenolA, whereas the curing agent is phenol-formaldehyde resin (Ciech Sarzyna S.A. Poland), and 2-ethyl-4-methylimidazole (Tokyo

Chemical Industry Co. LTD.) is used as catalyst. Graphene is supplied by Sigma Aldrich. Natural graphite NG–7 or acetylene black was supplied by Merck. Stoichiometric mixture of epoxy resin and novolac were combined using continuous stirring and heating up to 100 ºC. Epoxy precursor was cross-linked at different times (2-6 h) and temperatures (120 - 180 ◦C). Carbon foam was obtained in the process of self-foaming of previously prepared polymer precursor followed by the process of its carbonization at 900 ◦C in nitrogen atmosphere. The elemental analysis (EA) was performed on Vario Macro Cube (Elementar Analyzen systeme GmbH) equipment for determination of C, H, N, S. The combustion temperature for the system was 1150 ºC in an oxidizing atmosphere to form gaseous reaction products: CO_2, H_2O, N_2, SO_2. The individual gases are transported by a carrier gas to be measured by a thermal conductivity detector (TCD). Textural characterization of the samples was performed by using N_2 adsorption at 196 ◦C. Prior to the experiments, the samples were outgassed under secondary vacuum at 300 ◦C overnight. The N_2 adsorption isotherms were used to calculate the specific surface area, S_{BET} and pore volumes.

Results: Obtained samples (carbon foam, graphene, graphite) are characterized by XRD, Scanning Electron Microscopy, TG and DSC analysis, elemental analysis, and mechanical strength. Adding carbon fillers to foams affects, among other properties, their bulk density, thermal conductivity, mechanical properties and resistance to abrasion, crushing, and vibrations. The influence of the structure on the viscoelastic and friction properties of carbon composites is studied. The application of other porous carbon materials, namely, glassy carbon particles, to produce epoxy-carbon composites was studied, obtaining positive effects on the mechanical strength and electrical behavior of composites.

Conclusions: The results obtained demonstrate that the novel method, for producing carbon foam, using mixture of organic substances with suitable chemical properties and treatment conditions, allows avoiding the use of pressure and stabilization step, and enables the production of material with very good physico-chemical properties. The production of carbon foam by this method requires significantly less energy consumption, in comparison with usual synthesis methods.

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SECTION 1 - Multifunctional materials, nanocomposites, innovative technologies and cultural heritage preservation (Oral communications)

1. *BIO-BASED POLYBENZOXAZINE RESINS WITH POTENTIAL MEDICAL APPLICATIONS*
2. *EPOXIDIZED CORN OIL AN EFFICIENT POLYMER MATRIX FOR DEVELOPING ANTICORROSION NANOCOMPOSITE MATERIALS*
3. *CRYOSTRUCTURES AS POTENTIAL AGRICULTURAL FERTILIZERS WITH CONTROLLED RELEASE PROPERTIES*
4. *DETECTION OF ANALYTES (FROM PROTEINS TO BACTERIA) USING APTAMERS*
5. *MESOPOROUS SILICA MODIFIED WITH INORGANIC NANOPARTICLES AS CARRIERS FOR NATURAL COMPOUNDS*
6. *STUDY ON HYBRID SYSTEMS BASED ON TiO_2 FOR ENHANCING PHOTOCATALYSIS*
7. *USING ELECTROCHEMICAL BIOSENSORS FOR THE EVALUATION OF PLANT BIOSTIMULANT EFFECT – TACKLING CROP LOSS MITIGATION – with BIOSCREEN*
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9. *Synthesis And Characterization Of Donor-Acceptor Dyes For Organocatalyzed Atom Transfer Radical Polymerization (O-ATRP)*
10. *REPOSITIONING OF DES-FLUORO(6) QUINOLONES FROM ANTIMICROBIALS TO ANTIVIRAL DRUGS*
11. *CrSiCN BASED HARD-COATINGS USED FOR WOODWORKING APPLICATIONS*

BIO-BASED POLYBENZOXAZINE RESINS WITH POTENTIAL MEDICAL APPLICATIONS

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Keywords: bio-based benzoxazine, photothermal therapy, dendrimers, natural phenols

Introduction: The innovation of this research consists in developing new covalent functionalization routes to create the benzoxazine monomers directly on the proper chemically modified graphene oxide surface in order to obtain new exfoliated nanocomposite structures and to demonstrate their superior performance as compared with ordinary polybenzoxazines.

Materials and methods: To develop the novel nanocomposite structures, polyamidoamine (PAMAM) dendrimers were employed as functionalization agents for graphene oxide (GO), leveraging their terminal amino (-NH2) and carboxyl (-COOH) functional groups. Two types of PAMAM dendrimers with different generations were tested to determine the optimal conditions for modifying GO with a high content of benzoxazine groups. The modified GO was synthesized via the following process: amino groups on the GO surface were reacted with phenol and formaldehyde to create benzoxazine rings. These rings were subsequently polymerized to produce polybenzoxazine structures that incorporated exfoliated GO sheets within the polymer matrix.

Results: The dendrimer-assisted functionalization successfully grafted a high content of benzoxazine groups onto the GO surface, as verified through chemical analysis. PAMAM dendrimers of higher generation showed enhanced functionalization efficiency due to increased surface area and number of functional groups. The resulting GO-polybenzoxazine nanocomposites demonstrated improved exfoliation of GO sheets within the polymer matrix. These nanocomposites exhibited superior mechanical strength, thermal stability, and chemical resistance compared to ordinary polybenzoxazines. The incorporation of GO also contributed to enhanced biocompatibility, making the nanocomposites promising candidates for medical applications such photothermal therapy.

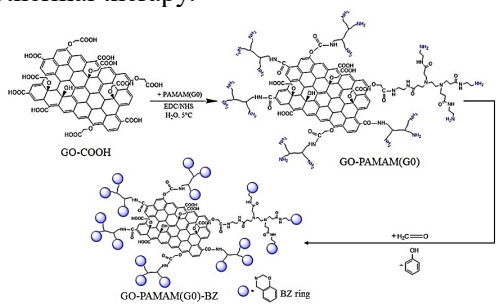

Fig. 1. Hyperbranched benzoxazine functionalized graphene oxide (GO-PAMAM-BZ)

Conclusions: This approach led to the formation of exfoliated GO-polybenzoxazine nanocomposites with significantly enhanced mechanical, thermal, and chemical properties compared to conventional polybenzoxazines. The use of dendrimers with varying generations allowed for optimization of the functionalization process, with higher-generation dendrimers yielding better performance [1].

***Acknowledgements**: This research study was supported by a National Research Grant - ARUT, contract no. 23/09.10.2023.*

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EPOXIDIZED CORN OIL AN EFFICIENT POLYMER MATRIX FOR DEVELOPING ANTICORROSION NANOCOMPOSITE MATERIALS

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Keywords: bio-based epoxy, nanohybrids, nanocomposites, protective coatings

Introduction: A great alternative to conventional epoxy monomers is the ones derived from vegetable oils. They have recently been employed for the development of sustainable networks with advanced performances [1]. Bio-based epoxy networks do not have the capability to stand corrosion by themselves, thus proper reinforcing with active nanofillers is required for such applications.
Materials and methods: The present work focuses on the development of hybrid nanoreinforcing agents based on functionalized graphene oxide and montmorillonite nanoclay that can further act as corrosion inhibitors. Considering the environmental concerns caused by the petroleum-based materials, epoxidized cord oil was used as polymeric matrix to synthesize nanocomposites. Extensive studies regarding the amine functional groups from the GO surface along with a range of nanoreinforcing ratio between 0.25 and 1% were done to assess the influence of nanohybrids within the coating materials.

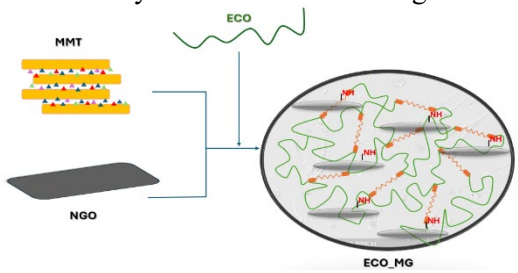

Figure 1 Schematic representation of the sustainable epoxy coatings synthesis

Results: Prior to nanocomposite development the chemical composition of the hybrid nanostructures was first confirmed by FTIR and XPS analysis. Thermomechanical properties of the final nanocomposites were evaluated and correlated with the structure of the hybrid nanostructures by dynamic mechanical analysis (DMA) and thermogravimetric analysis (TGA), showing a great influence even at low concentrations. The impact of the chemical particularities of each hybrid nanomaterial over the curing process of the polymeric matrix was evaluated through differential scanning calorimetry (DSC). The surface properties of the final materials were characterized in terms of contact angle measurements and the anticorrosion performances were evaluated through salt spray test.

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CRYOSTRUCTURES AS POTENTIAL AGRICULTURAL FERTILIZERS WITH CONTROLLED RELEASE PROPERTIES

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Keywords: chitosan, cryostructures, organic waste, liquid digestate, fertilizers

Introduction: The global population is expected to exceed 9 billion by 2050 and therefore current agricultural practices cannot meet the growing demand for food without extensive application of fertilizers. However, conventional fertilizers are inherently limited by low nutrient use efficiency, so the agricultural sector will have to ensure food security without harming the environment. Modern technology will also be required in agro-ecosystems to assure enough food production and to reduce the harmful environmental effects brought on using chemical fertilizers [1-2]. Numerous studies in literature have focused on the development of controlled release biofertilizers. Nitrogen (N), phosphorus (P) and potassium (K) are essential nutrients for plant growth. However, the application of these nutrients in the form of chemical fertilizers affects crops and soil [3]. Which is why, controlled release of nutrients is need. This technology allows controlled release of nutrients into the soil, providing a sustainable solution for fertilizing agricultural crops. This approach is an important step towards improving the efficiency of the global food system and protecting the environment. By using composite materials with controlled nutrient release capacity, it can reduce dependence on chemical fertilizers and minimize pollution of soil and water resources, thus contributing to a healthier environment and more sustainable agriculture [4].

Materials and methods: For the preparation of innovative composite cryostructures with a significant nutrient content, commercial chitosan (CC) and liquid digestate (obtain from anaerobic digestion of organic waste) were used. Other reagents: acetic acid, was used in mixture with water, for chitosan dissolution; and a foaming agent to obtain a supermacroporous structure. Two series of samples were prepared, some based on chitosan being considered as reference samples and in the case of the second series there were also nutrient-containing cryostructures.

Results: With the aim of highlighting the properties of the aimed materials, several characterization techniques were needed (FTIR, SD, SEM and ICP-OES). The FTIR spectra confirmed the incorporation of the liquid digestate into the polymer matrix, by the appearance of the characteristic bands for the materials. The Swelling Degrees were studied at three different values of pH (4,7 and 9) to establish the behavior of the samples. Following this study, the cryostructures were able to adsorb significant amount of N, P and K. In the end the cryostructures with liquid digestate content were studied in terms of their controlled release capacity (of N, P and K) by ICP-OES.

Conclusions: In conclusion, new composite cryostructures based on chitosan and liquid digestate were developed. These materials show great properties in terms of their structure, morphology and swelling capacity, making them potential candidates for future agricultural applications, as well as controlled release systems for NPK.

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DETECTION OF ANALYTES (FROM PROTEINS TO BACTERIA) USING APTAMERS

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Keywords: aptamer, bacteria, biosensor, magnetic particles

Introduction: Aptamers are molecules that can bind to a specific target with high specificity recognizing a wide palette of analytes. Being effective and practical, we investigated the use of aptamers for recognizing two of the main analytes in nature: proteins and bacteria. For proteins we create an amplification system in which a sandwich type of biosensor for lysozyme would be used on a microarray plate, starting from an aptamer for lysozyme which was labeled with a cold active aldehyde dehydrogenase from the Antarctic Flavobacterium PI002 (F-ALDH). For bacteria, we tested an assay based on magnetic particles (MP) *S. typhimurium* aptamer was bound. The assay is used to specifically capture and detect S. typhimurium bacteria.

Materials and methods: We created a complex based on the histidine tag of the FALDH that exhibits affinity for the nickel-Nα, Nα-Bis(carboxymethyl)-L-lysine hydrate complex**.** Then, starting from a microarray plate where lysozyme was absorbed on the wells, the complex was bound to the lysozyme based on the specificity of the aptamer. We also tested an assay based on the *S. typhimurium* aptamer for the detection of Salmonella bacteria using streptavidin modifies MP.

Results: The successful attachment of F-ALDH to the aptamer was verified by checking the absorbance values at 260 nm and 280 nm in the UV spectrum. We confirm the bounding of the complex to the lysozyme by measuring the enzymatic activity of the wells where the complex was incubated and the lack of enzymatic activity of the wells where FALDH was incubated as a blank.

Also, A quantitative method based on fluorescence was developed for evaluating the number of bacteria that were captured using the aptamer -MP assay. Also, the formation of MP-bacteria specific cluster was observed using fluorescence microscopy.

Conclusions: Protein-aptamer of the complexes were obtained and characterized successfully. Further tests are envisaged to characterize the entire complex. Bacteria-MB cluster formation was validated using fluorescence microscopy while the capture ability of the modified MP was characterized using a new developed method based on fluorescence.

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MESOPOROUS SILICA MODIFIED WITH INORGANIC NANOPARTICLES AS CARRIERS FOR NATURAL COMPOUNDS

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Keywords: mesoporous silica, inorganic nanoparticles, phenolic compounds, encapsulation, antioxidant activity

Introduction: Functionalized mesoporous silica has been widely studied as carrier either for drugs or phytocompounds due to its capacity to accommodate large amounts of organic molecules, high biocompatibility, and surface properties that can be tuned through functionalization with organic moieties or inorganic nanoparticles (NPs) [1,2]. Among phytocompounds, phenolic substances stand out due to their anti-inflammatory, antioxidant, and antibacterial properties [3]. The objective of this study was to obtain mesoporous silica spheres modified with inorganic nanoparticles in order to be applied as carriers for wild bilberry leaf extracts.

Materials and methods: Pristine and functionalized mesoporous silica obtained by sol-gel method was modified with ZnO, Cu or noble metal NPs. The resulting composite materials were characterized by X-ray diffraction, FTIR spectroscopy, SEM, N_2 adsorption-desorption isotherms, and thermal analysis. The cytocompatibility and antioxidant activity of resulting composite materials were assessed on HaCaT keratinocytes cell line.

Results: Mesoporous silica modified with inorganic particles exhibited high porosity, being able to accommodate into the mesopores in the range of 37-40.2% (wt) polyphenols from extract. In the case of mesoporous silica spheres modified with inorganic NPs, ZnO nanoparticles, in amorphous state, were distributed inside the silica spheres, while copper, silver or gold nanocrystals were present also on the silica surface. The incorporated extract exhibited good biocompatibility up to 50 μg/mL dose of treatment and higher antioxidant activity than the free extract on HaCaT keratinocytes cell line. The chemical profile of the wild bilberry leaf extracts was determined by spectrometric determinations of total polyphenols and flavonoids content, as well as by reverse phase high performance liquid chromatography. The main components of prepared polyphenolic extracts were rutin hydrate and chlorogenic acid, which are well known for their benefits for human health.

Conclusions: A synergistic antimicrobial effect between inorganic NPs and bilberry leaves extract was observed against standard *Staphylococcus aureus* (ATCC 25923) strain. Based on their biocompatibility and antioxidant activity, the prepared composite materials can be used for topical applications.

***Acknowledgements**: The financial support from UEFISCDI (Romania) through project PCE no. 117/2022 is highly appreciated.*

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STUDY ON HYBRID SYSTEMS BASED ON TiO_2 FOR ENHANCING PHOTOCATALYSIS

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Keywords: photocatalyst, heterojunction, dye removal, titanium dioxide

Introduction: Titanium dioxide (TiO_2), a semiconductor with excellent optical and electrical properties, faces low photocatalytic activity due to issues like fast recombination, limited electron mobility, and restricted optical absorption. Designing appropriate heterojunctions is proved to be a promising method to address most of these issues and thus to improve the photocatalytic performance [1]. The present work reports the synthesis of TiO_2 photocatalysts with metal-oxide heterojunctions. The technology has been applied for the purification of water effluents contaminated by the industrial dye reactive yellow 176.
Materials and methods: The photocatalytic nanoparticles were synthesized using a chemical microwave technique, combining TiO_2 with metal oxide precursors like cobalt, copper, manganese, and chromium acetates, along with ferric chloride, resulting in a hybrid photocatalyst. The synthesis of metal oxide heterostructures was achieved with a Discover 2.0 Microwave Reactor at 160°C. The acquired samples were characterized using relevant analytical techniques to verify that the photocatalysts exhibited the requisite qualities. The photocatalytic characteristics of the produced materials were evaluated by individually combining the metal-oxide photocatalysts with a styrene-acrylic film-forming compound. The performance of the composites was comparatively assessed in the photocatalytic degradation of Drimaren yellow CL-2R dye from aqueous solutions under arc-xenon irradiation, while chromophore degradation was monitored via UV-Vis absorption spectroscopy [2, 3].
Results: The developed photocatalysts were evaluated using FTIR, XRD, BET, TGA and EDX analyses. The doping ratio and the duration of UV light were identified as the two critical elements influencing the synthesis process.

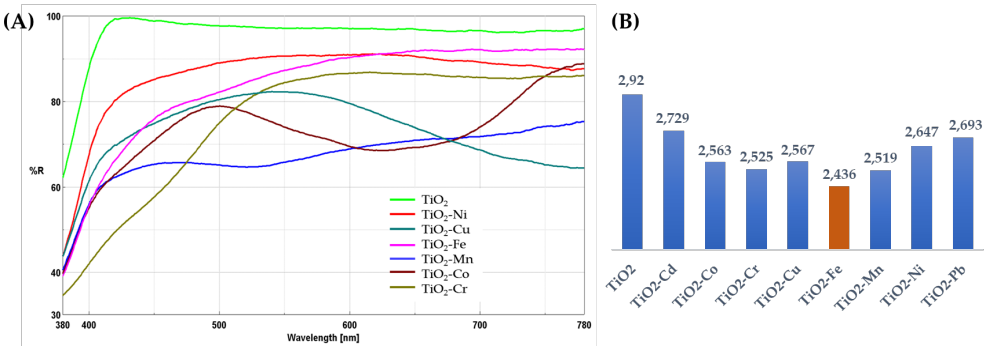

Figure 1. **(A)** UV-Vis diffuse reflectance spectra and **(B)** band-gap energy values of the synthesized photocatalysts.

Conclusions: New photocatalytic nanocomposites were synthesized by a straightforward chemical method including the formation of metal oxides on the surface of TiO_2 nanoparticles via the hydrolysis of the precursor under microwave irradiation. The efficiency of degradation depends on the quantity of active radicals and the duration of the photocatalytic process. The most effective results were achieved by TiO_2/Fe_2O_3, wherein nanometric TiO_2 particles are deposited onto the surface of micrometric Fe_2O_3 particles.

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Projects to finance excellence in RDI, Contract no. 15PFE/2021 and INCDCP-ICECHIM Core program PN 23.06.01.01 (AQUAMAT).

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USING ELECTROCHEMICAL BIOSENSORS FOR THE EVALUATION OF PLANT BIOSTIMULANT EFFECT – TACKLING CROP LOSS MITIGATION – with BIOSCREEN

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Keywords: metal phthalocyanines, peroxynitrite, biostimulants, biosensors, crop loss

Introduction: According to FAO (Food and Agriculture Organization), food demand will increase by 50% until 2050 and 80% of the food demand is based on plant products. In contrast, up to 40% of the scarce natural resources are due to crop loss, which translates into a loss of $220 B. Understanding how crop loss occurs, helps understanding how crop loss can be mitigated: the three phases of crop loss hide behind the curtains the invisible signaling of plant damage performed by the Reactive Oxygen Species (ROS). If we take a closer look into the "invisible bad phase", we can observe how ROS act like frenemies (both a friend and an enemy, under certain circumstances) through redox signaling in plants [1]. Crop loss mitigation could be achieved by using fast, wearable, remote redox sensors, that can read what happens during this "invisible bad phase", through early and real-time detection for real-time decision making among farmers or different interested stakeholders (such as applying different agrochemicals or watering plants). As biostimulants are agrochemicals defined by any substances/microorganisms applied to plants with the aim to enhance nutrition efficiency, efficient biostimulants will also mitigate abiotic stress in plants, when plants actually need them [2].

Materials and methods: Cyclic Voltammetry (CV), Chronoamperometry (CA), FTIR, SEM, UV-Vis, Fluorescence Spectroscopy, *in-vitro* growth of model plants in presence/absence of stressor (such as *Arabidopsis Thaliana* and *Vigna radiata,* ± $CdCl_2$), accumulated fresh biomass determination, determination of pigments and antioxidant activity, Quantic Yield (QY), XRF etc. Materials such as metal phthalocyanines (MPc) and screen-printed carbon electrodes (SPCE) were used to develop the electrochemical sensors.

Results: In this work electrochemical ROS sensors were developed for the direct oxidative stress determination, correlated with the determination of biostimulant effects of three commercial biostimulants: lower electrochemical signal in the presence of biostimulant is correlated with a higher biostimulant effect. The efficiency order of biostimulants was correlated with the other methods described.

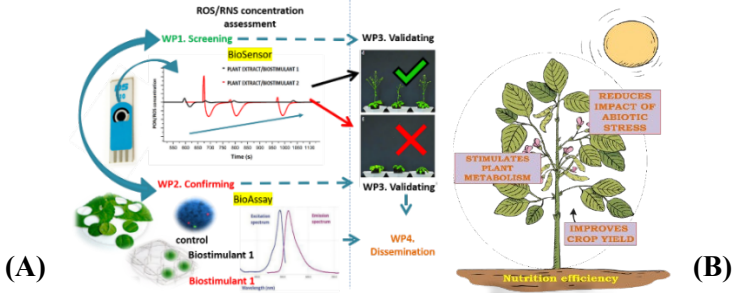

Figure 1. (A) The correlation between different BioScreen project work packages and the methods/approaches used. (B) The visual representation of biostimulants.

Conclusions: The developed processes and methods are efficient for peroxynitrite detection and the best ones were used for screening biostimulants (WP1). The best method was compared with the validation method (applying the best biostimulants for growing plants, WP3) and the confirming method (fluorescence, WP2). Integrating these sensors into health monitoring devices for plant care could tell us when plants need saving!

***Acknowledgements**: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS - UEFISCDI, project number PN-III-P1-1.1-PD-2021-0798, within PNCDI III, contract number PD116/2022. The authors also gratefully acknowledge the support of the Ministry of Research, Innovation and Digitization through the PN 23.06 Core Program - ChemNewDeal within the National Plan for Research, Development and Innovation 2022-2027, developed with the support of Ministry of Research, Innovation, and Digitization, project no. PN 23.06.01.01 AquaMat.*

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Biomimetic PEGDA-based Nanogels for the Recognition and Binding of Spike S1 Protein from SARS-CoV-2

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Keywords: nanogels, protein binding, cytotoxicity, Spike S1 RBD, molecularly imprinted polymers

Introduction: The global COVID-19 pandemic has encouraged extensive research into new approaches for detection and treatment. A favorable alternative which has been taken into consideration is the development of synthetic antibodies that selectively target the Spike S1 protein from SARS-CoV-2 virus, which facilitates the virus's entry into host cells [1]. Nanogels (NGs) are nano-sized particles formed from a crosslinked polymer network (10-300 nm) which can be tailored to possess desirable characteristics such as high-water content, biocompatibility, and responsiveness to external stimuli [2]. This type of material has a wide range of potential applications in fields such as drug delivery, tissue engineering, and biosensing, due to their ability to encapsulate and release therapeutic agents in a controlled manner, as well as their ability to mimic natural biological structures [3]. Among synthetic materials, molecularly imprinted polymers (MIPs) stand out for their ability to achieve high specificity and sensitivity toward target molecules [4]. This study focuses on synthesizing MIP nanogels (MIP-NGs) by imprinting the 3D structure of the Spike S1 receptor-binding domain (RBD) within a nanohydrogel matrix. These molecular imprints create affinity sites for the selective rebinding of the Spike S1 protein, effectively mimicking the behavior of natural antibodies.

Materials and methods: The MIP-NGs were obtained by reverse miniemulsion polymerization of polyethylene glycol diacrylate (PEGDA) as macromonomer in presence of SARS-CoV-2 Spike S1 protein RBD (PSS1) as a template molecule. Control NGs were prepared without PSS1.

Results: Characterization of NGs was carried out using different techniques such as FTIR, TGA/DTG, DLS, TEM and SEM. FTIR and TGA/DTG analyses confirmed the extraction of both emulsifiers and template from the MIP-NGs, while DLS and SEM/TEM images highlighted the individual spherical structures of the synthesized NGs which also maintained their size below 300 nm. The binding study expressed by adsorption efficiency and rebinding capacity of the MIPS and NIPs towards PSS1 was carried out using UV-Vis spectroscopy (Bradford method) and SDS-PAGE, while the cytotoxicity was evidenced by MTT assays. These analyses indicated that the MIP-NGs exhibited higher binding affinity for PSS1 compared to the control NGs, as well as high cellular viability in 72 hours at various dilutions.

Conclusions: In summary, the morphological and structural characterization of the samples confirmed the presence of the compounds of interest and indicated the desired size for the potential application. MIP-NGs exhibited high specificity and binding affinity for PSS1, making them promising candidates for synthetic antibody development. Additionally, MIP demonstrated excellent biocompatibility, making them suitable for potential in vivo applications.

Acknowledgements: *The research group from ICECHIM gratefully acknowledges the financial support from UEFISCDI, through the supporting project PN-III-P1-1.1-TE-2021-1239 grant no. 144/2022 (ANTISPIKE), and from the Ministry of Research, Innovation and Digitalization, through the institutional ctr. no. PN 23.06.01.01 (AQUAMAT).*

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Synthesis And Characterization Of Donor-Acceptor Dyes For Organocatalyzed Atom Transfer Radical Polymerization (O-ATRP)

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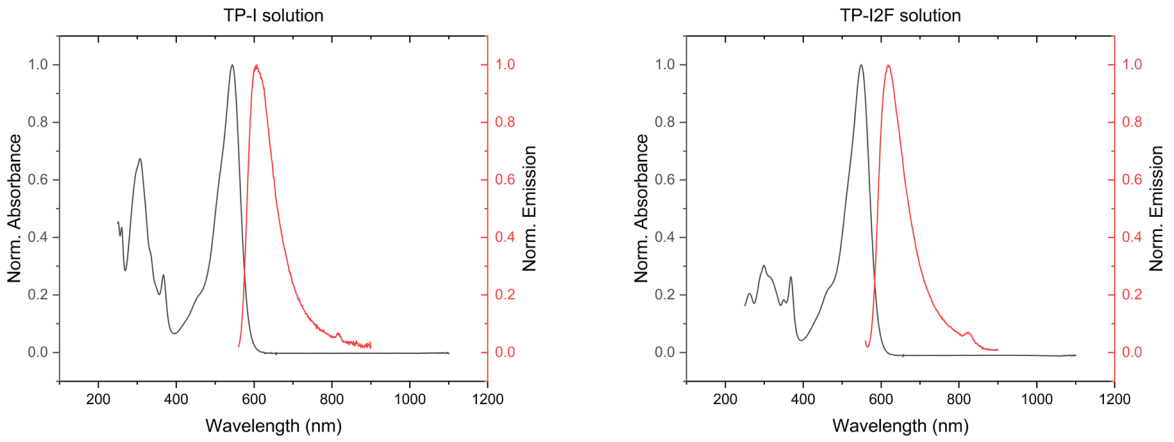
Introduction: Following the seminal report in the mid-1990s [1], Atom Transfer Radical Polymerization (ATRP) became a staple in the controlled radical polymerization (CRP) field.
Materials and methods: ATRP offers excellent control over final product molecular weight and polydispersity index, with a big pool of possible monomers. Conventionally, ATRP employs transitional metal salts, mainly copper (I), as catalysts to modulate the concentration of the propagating radicals through the formation of persistent radicals [2] in the system. Their presence in the final polymer is problematic to some industrial sectors since they can be poisonous at very low concentrations. Plenty of effort went into lowering the heavy metal contents of the final product by either reducing the initial quantity of catalyst during polymerization or by better and more sophisticated purification methods [3]. However, these techniques do not fully remove the transitional metals from the formulation. Since the early 2010s, metal-free CRPs have received increased attention from researchers. Photoinduced organocatalyzed ATRP (O-ATRP) offers the desired control on the molecular weight and polydispersity indexes, the extensive monomer variety, without using heavy metals in the polymerization technique [4]. The discovery of O-ATRP opened possible applications in areas lacking conventional ATRP, such as biomedical, electronic, packaging, etc. Herein, we investigate the synthesis and characterization of two donor-acceptor (D-A) push-



pull dyes that will be used in the future for O-ATRP.
Results: Both dyes have been shown to have absorption maxima in the visible region, at 544 and 549 nm, making them good candidates for conducting photocatalysis in natural light.

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REPOSITIONING OF DES-FLUORO(6) QUINOLONES FROM ANTIMICROBIALS TO ANTIVIRAL DRUGS

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Keywords: drug design, molecular docking, antimicrobials, antiviral drugs

Introduction: Quinolone derivatives represent one of the extensively utilized antimicrobial drugs. Quinolone derivatives also have other biological activities: antitumor activity, antimycobacterial activity and antiviral activity. From quinolone derivatives with antiviral activity. The first quinolone integrase inhibitors drug, approved by the U.S. Food and Drug is Elvitegravir (6-[(3-chloro-2-fluorophenyl)methyl]-1-[(2S)-1-hydroxy-3-methylbutan-2-yl]-7-methoxy-4-oxo-quinoline-3-carboxylic acid [1]. In previous research [2], a series of non-fluorinated quinolones were synthesized. These compounds showed a low antimicrobial activity. In this work, computational studies are presented, to identify which compounds could present inhibitory activity against HIV-1 reverse transcriptase (RT).

Materials and methods: For six des-fluoro(6)-quinolones have been performed molecular modeling studies using Spartan'24 software [3]. The docking studies have been conducted using CLC Drug Discovery Workbench Software [4] and Molegro Virtual Docker Software [5] to predict the binding modes, the binding affinities, and the orientation of the docked quinolones in the preferred binding site of the protein receptor.

Results: In this study, the DFT/B3LYP/6-311G* level of basis set has been used for the computation of molecular structure, vibrational frequencies, and energies of optimized structures. The score and hydrogen bonds formed with the amino acids from group interaction atoms are used to predict the binding modes, the binding affinities and the orientation of the docked quinolone compound in the active site of the protein-receptor (Figure 1,2). The protein-ligand complex has been realized based on the X-ray structure of *HIV-1 Reverse Transcriptase (RT)*, who was downloaded from the Protein Data Bank (PDB ID: 2ZD1).

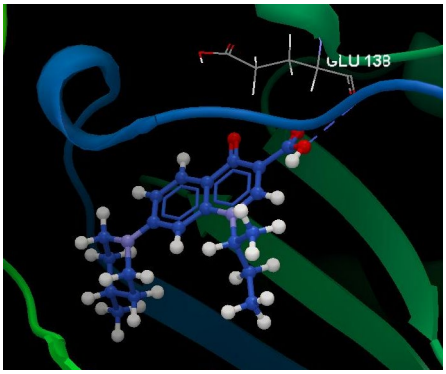

Figure 1. Hydrogen bond (blue dotted lines) between HPQ31 and amino acid residue from binding site of 2DZ1 receptor

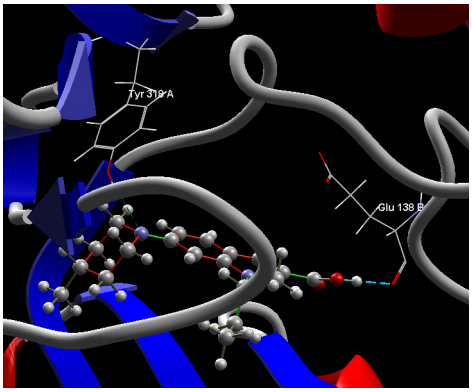

Figure 2. Hydrogen bond (blue dotted lines) between HPQ31 and amino acid residues from binding site of 2DZ1 receptor

Conclusions: Computational investigations have shown the non-fluorinated quinolones have the potential to inhibit HIV-1 reverse transcriptase (RT).

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CrSiCN BASED HARD-COATINGS USED FOR WOODWORKING APPLICATIONS

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Keywords: CrSiCN coatings, mechanical properties, corrosion resistance, woodworking applications

Introduction: Woodworking applications represent a rapidly expanding field focused on developing advanced coatings with enhanced wear resistance, reduced friction, and efficient corrosion protection [1]. Chromium silicon carbonitride (CrSiCN) coatings have emerged as a promising solution, offering a unique combination of properties suitable for various industrial uses [2]. The C/N ratio plays a crucial role in influencing the coatings' mechanical and tribological performance. This research explores how optimizing the C/N ratio can improve the functionality of CrSiCN coatings, making them more durable, efficient, and long-lasting in demanding environments.

Materials and methods: The coatings were deposited using a reactive cathodic arc evaporation unit equipped with a CrSi cathode. The CrSiCN layers were investigated for elemental and phase composition, microstructure, mechanical properties, corrosion resistance, and tribological behavior. Morphology and composition measurements were performed before and after corrosion and tribocorrosion tests.

Results: Adhesion enhancement was observed with an increase of C_2H_2 flow rate, while reducing the flow rate of N_2 gas (Fig.1). C50N50 composition proved the best wear performance in the case of each investigated substrate, making it an excellent choice for applications where wear resistance is critical. Also, the C70N30 sample showed the highest wear rate, signifying that it may be less suitable for applications with high wear requirements (Fig.2). The results showed that the C/N ratio is a critical parameter, the coatings with higher carbon content presented slightly enhanced corrosion resistance, being able to withstand similar real-life operating conditions. CrSiCN C30N70 coating on the S1 substrate consistently exhibited the best corrosion resistance among the investigated samples.

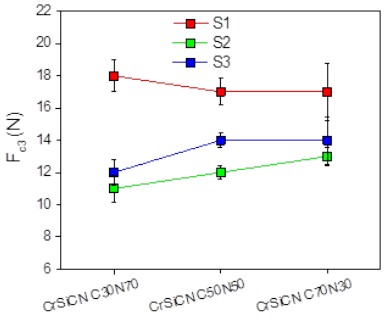

Figure 1. Evolution of the critical force (Fc3) for complete coating delamination

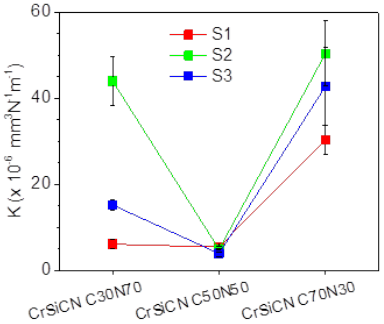

Figure 2. Wear rate, K, for CrSiCN coatings deposited on S1-S3 substrates

Conclusions: The findings demonstrate that the final properties can be fine-tuned by selecting specific deposition conditions. In particular, coatings with higher carbon content exhibited improved corrosion resistance, enabling them to endure operational conditions akin to real-life scenarios.

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SECTION 1 - Multifunctional materials, nanocomposites, innovative technologies and cultural heritage preservation

(Poster presentations)

1. *PLASTIC WASTE DERIVED CARBON/CARBON COMPOSITES FOR CONSTRUCTION OF ROCKET COMPONENTS*
2. *SYNTHESIS OF ECO-FRIENDLY SILVER NANOPARTICLES USING WILD GARLIC (ALLIUM URSINUM) LEAVES EXTRACT AND THEIR ANTIMICROBIAL ACTIVITY*
3. *THE DEVELOPMENT AND APPLICATION OF NANOCOMPOSITE MATERIALS FOR THE PRESERVATION AND CONSOLIDATION OF CULTURAL HERITAGE*
4. *MORTAR COMPOSITIONS BASED ON SPENT MUSHROOM SUBSTRATE*
5. *RADIATION-INDUCED DEGRADATION OF POLYMERIC INSULATORS: A KINETIC MODEL FOR LIFETIME ASSESSMENT*
6. *IDENTIFICATION OF THE DEPENDENCE BETWEEN THE SHAPE OF ELECTRODES FOR PROCESSING METAL SURFACES THROUGH ELECTRIC DISCHARGES AND THEIR WEAR*
7. *SYNTHESIS, ANTIBACTERIAL, ANTIOXIDANT AND ADME STUDIES OF SOME PYRIMIDINE COMPOUNDS*
8. *ADVANCED HYBRID MATERIALS BASED ON NATURAL POLYMERS: A NEW REMEDIATION STRATEGY FOR WATER CONTAMINATED WITH HEAVY METALS*
9. *RELEASE KINETICS OF CURCUMIN FROM MICROBIAL POLYMERS BASED NANOSYSTEMS*
10. *DESIGN AND ANALYSIS OF AN INNOVATIVE ENZYMATIC-FILTER (E.F.) FOR PURIFYING AIR CONTAMINATED WITH SULFUR DIOXIDE (SO_2)*
11. *WEARABLE MULTISENSING PATCH BASED ON SWCNT-PtNPs NANOCOMPOSITE FOR CLINICAL BIOMARKERS MONITORING FROM SWEAT*
12. *MARBLE DEGRADATION ASSESSMENT VIA SALT CRYSTALLIZATION METHOD*

PLASTIC WASTE DERIVED CARBON/CARBON COMPOSITES FOR CONSTRUCTION OF ROCKET COMPONENTS

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Keywords: carbon composites, household waste, disposable packing

Introduction: C/C composites are distinguished by unique properties: high specific strength, low density, low coefficient of thermal expansion, very good mechanical properties at high temperature, good ablation resistance. Mixtures of household waste containing polypropylene, polyethylene, nylon66, polystyrene (disposable food packaging and cups) are used as precursors for preparation of carbon composites.

Materials and methods: The mixed waste is heated up to 200 °C until melting, 10 cm^3 98% $H_2SO_4$is added by drops to the reaction mixture with continuous stirring until solidification. The resulting solid product was heated up to 750 °C in a reactor with a heating rate of 10 °C min^{-1} under an inert N_2 atmosphere. The final product is ground into a fine powder which is mixed with heat insulation polystyrene waste, homogenized well and the mixture is poured into a mold which is pressurized up to 25 atm. After removal from the mold, the composite was heated in an inert N_2 atmosphere up to 850 °C with a heating rate of 5 °C min^{-1}.

Results: The obtained samples were characterized by modern techniques like XRD, BET, SEM etc.

Conclusions: The obtained materials will be applied further for construction of components in solid propellant rockets.

***Acknowledgements**: The authors acknowledge funding provided by Romanian-Bulgarian Academy Joint Project INNOMAG (2022-2024), in the frame of collaboration between Romanian Academy of Sciences and Bulgarian Academy of Sciences.*

SYNTHESIS OF ECO-FRIENDLY SILVER NANOPARTICLES USING WILD GARLIC (*ALLIUM URSINUM*) LEAVES EXTRACT AND THEIR ANTIMICROBIAL ACTIVITY

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Keywords: plant extract, LC-MS, XRD, antimicrobial activity

Introduction: The emergence of metallic nanoparticles through green synthesis has obtained a significant recognition in the last decade and the global research efforts which utilised eco-friendly practices has often termed as the green revolution (1,2). This research presented the use of wild garlic leaves (*Allium ursinum)* for the biosynthesis of silver nanoparticles with enhanced antioxidant and antibacterial properties. Being a medicinal plant, wild garlic is a perennial belonging to the *Allium* family, which has a rich phytochemical content and offer a multifaceted approach to combating oxidative stress and cancer (3). The most important chemical constituents with pharmacological activity of wild garlic are sulfur compounds (sulfoxides). Also, their leaves apport an important source of methiin, alliin, alkaloids, polyphenolic and flavonoids compounds (4), useful for different types of diseases: gastrointestinal, cardiovascular, respiratory (5,6).
Materials and methods: The wild garlic extract and synthesized nanoparticles were characterized by ultraviolet–visible (UV–Vis) and Fourier-transform infrared (FT-IR) spectroscopy, Liquid chromatography–mass spectrometry (LC-MS) and gas-chromatography (GC), X-ray diffraction (XRD) analysis and transmission electron microscopy (TEM) techniques.
Results: The antimicrobial activity of the synthesized nanoparticles (AgNPs) and wild garlic (WG) extract were studied against some bacteria and fungi using the disk diffusion method. The AgNPs-WG were highly effective against the tested pathogenic microorganisms. The diameter of the inhibition zone by the silver nanoparticles against *S. Aureus* was measured to be 22 mm, almost equal to the result obtained using C. *Albicans* (21.5 mm). FTIR and UV-Vis analyses confirmed the reduction of Ag (I) to Ag (0) in the presence of wild garlic leaves extract. Also, the wild garlic extract and AgNPs-WG presented good results for antioxidant activity.
Conclusions: In this research, silver nanoparticles were synthesized during a simple and green method mediated by the wild garlic (*Allium Ursinum*) leaves. The first step of this research, was to evaluate its morphological characteristics of wild garlic (*Allium ursinum*) leaves extract and its antioxidant and antimicrobial properties. Because the results revealed that *Allium ursinum* can be considered a valuable source of bioactive compounds, it was obtained silver nanoparticles in presence of this plant, and were characterized.

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THE DEVELOPMENT AND APPLICATION OF NANOCOMPOSITE MATERIALS FOR THE PRESERVATION AND CONSOLIDATION OF CULTURAL HERITAGE

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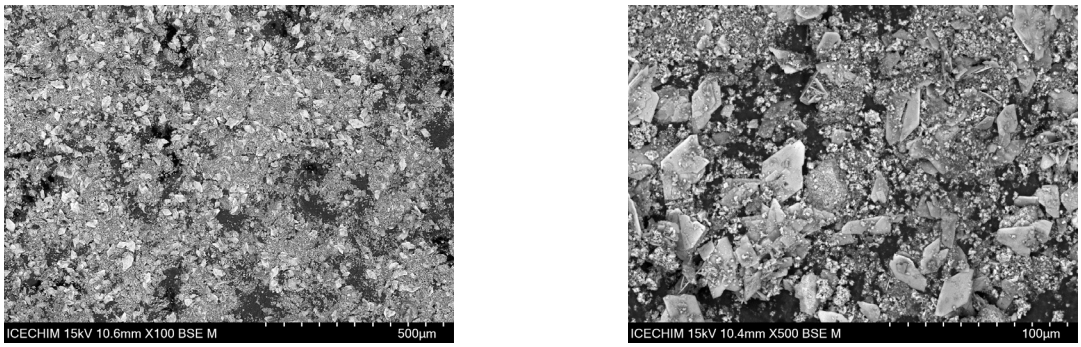
Keywords: consolidation, hydrophobic material, cultural heritage, nanocomposite materials

Introduction: Cultural heritage holds significant importance as it embodies human identity and offers a record of existence and activities throughout history. It encompasses both tangible artifacts and intangible qualities passed down through generations within a society or group. Acting as a link between the past and the future, cultural heritage demands specific preservation efforts in the present. Due to its inherent value to communities, safeguarding cultural heritage is crucial to ensure it endures for the benefit of future generations. Tangible cultural heritage is especially vulnerable to degradation or destruction, a process that has accelerated in recent years due to increasingly severe and frequent environmental conditions. The causes of cultural heritage deterioration can be grouped into two main categories: natural factors and anthropogenic factors [1-4]. Various apatitic materials and nanocomposite materials have been formulated for the treatment of natural or artificial stone artifacts of vernacular constructions and model artifacts on inorganic supports have been developed for the application of these materials

Materials and methods: The apatitic materials substituted with heavy metals were morpho-structurally characterized by modern techniques (XRD, XRF, FTIR, TGA, SEM) and the nanocomposite materials were morphologically characterized by SEM-EDX. After the developed materials were applied to the model artifacts, different hydrophobicity and mass variation tests were performed and the aesthetic parameters were evaluated through color tests

Results and conclusions: The hydrophobicity tests confirmed that the nanocomposites developed exhibit a strong hydrophobic character when applied to the model artifacts. By weighing the artifacts before and after treatment, it was proven that the nanocomposites do not alter the underlying material. Additionally, color tests showed no significant aesthetic changes following the treatment.



SEM image for the multilayered nanocomposite material composed of Hydrotalcite/TiO_2/ZnHAP/$Ca(OH)_2$

***Acknowledgements**: The authors gratefully acknowledge the support of the Ministry of Research, Innovation and Digitization through the PN 23.06 Core Program - ChemNewDeal within the National Plan for Research, Development and Innovation 2022-2027, developed with the support of Ministry of Research, Innovation, and Digitization, project no. PN 23.06.01.01 AquaMat.*

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MORTAR COMPOSITIONS BASED ON SPENT MUSHROOM SUBSTRATE

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Keywords: spent mushroom substrate, mortar, construction material, polymer coating

Introduction: Spent substrate resulting from mushroom cultivation (SMS) is a residual lignocellulosic material, mainly composed of sawdust, generated after collecting the fungi. About 5 kg of sawdust are used for each kg of cultivated mushrooms. The improper disposing or reuse of SMS contribute to environment pollution (soil, water and air contamination). Thus, it is necessary to find recycling methods for this main by-product of the mushroom cultivation process, and reduce the consequences regarding the serious environmental problems and financially demanding. SMS compost found uses as fertilizer for plant growth and for improving health, nutrients amount and water retention capacity of soil [1,2]. Among these possibilities, including spent mushroom substrate into mortars' composition can be considered as a suitable technique for reducing the waste amount, with resulting lightweight, ecological mortars.
Materials and methods: The studied mortars were composed by: usual cement used for internal and external strength structures, sand, water, and 5-40% SMS (as reported to sand). The variation of water amount required to obtain the same consistency of the mortar with the amount of SMS was observed, due to the affinity of this material for water. Since a decrease in the strength of the hardened mortar was observed when higher amounts of SMS were used, the samples were covered by a polymer-SMS coating. Mortars strength, resistance to decay and hydrophobicity were tested.
Results: The study represents an alternative for obtaining mortars for different applications in the construction field, which do not require high strength properties. The use of this wood waste offers opportunities to obtain materials with a lower density that can reduce the load supported by the building structure/foundation, with possible anti-sound or insulation properties. By covering the surface of this mortar, the resistance to degradation under the action of atmospheric water and precipitation can also be improved.

Figure 1 Aspect of specimens obtained from SMS mortar without covering (a), and SMS-polymer coated mortar (b)

Conclusions: The complete characterization of mortars containing spent mushroom showed that up to 20% SMS can be used to result low density and modest variations in properties in terms of mechanical and decay resistance, as well as hydrophobicity, especially by coating with the polymer solution.

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RADIATION-INDUCED DEGRADATION OF POLYMERIC INSULATORS: A KINETIC MODEL FOR LIFETIME ASSESSMENT

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Keywords: DSC, Onset Oxidation Time, Onset Oxidation Temperature, kinetic model, lifetime assessment

Introduction: The durability of polymeric materials is intrinsically tied to their degradation under specific operating conditions. This degradation occurs when multiple stressors-such as high temperatures, sunlight, ionizing radiation, solvents, or mechanical stresses-act simultaneously. For electrical cables, which play a vital role in electricity transmission, automation, control systems, and data communication, the durability of electrically insulating materials is critical for ensuring the safety and reliability of industrial, research, transportation, and domestic activities.

Materials and methods: Polymeric materials: cable insulators and external jackets made from materials such as LDPE (Low-Density Polyethylene), HDPE (High-Density Polyethylene), XLPE (Cross-Linked Polyethylene), and EVA (Ethylene Vinyl Acetate) that were irradiated at various doses during the operation, for over 5 years, of the Large Hadron Collider (LHC) machine at CERN (Fig. 1). These materials were exposed to radiation to assess their long-term durability and performance in the extreme conditions of the LHC. To measure the degradation and stability of these polymers, Differential Scanning Calorimetry (DSC) was utilized, specifically analyzing the OIT (*Onset Oxidation Time*) and OOT (*Onset Oxidation Temperature*) values.

Results: This study focuses on the aging of various electrically insulating materials, particularly polymers used in electrical cables within particle acceleration systems at CERN (e.g., LHC, SPS). Additionally, a simplified kinetic model was developed to simulate the degradation processes under the unique operating conditions at CERN, where ionizing radiation fields vary significantly in intensity (flux and energy) over time. The kinetic model, tested on dozens of CERN cables, was primarily based on the exponential depletion of antioxidants in polymeric insulation, as measured by Differential Scanning Calorimetry (DSC), particularly through Oxidation Induction Time (OIT, Fig. 2 [1]) and Onset Oxidation Temperature (OOT).

Fig. 1 – Cable witnesses exposed in real conditions of use (CERN- LHC)

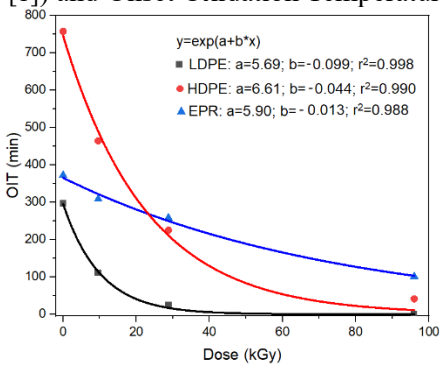

Fig. 2 - Typical exponential decrease in OIT values with irradiation dose. OIT values were isothermally recorded at 190 °C (LDPE) and 200 °C (HDPE and EPR).

Conclusions: The kinetic model's practical value lies in its adaptability to a broader range of operating conditions and materials, enabling more accurate diagnostics of degradation and assessment of the remaining service life.

***Acknowledgements**: The financial support was provided by Ministry of Research, Innovation and Digitization, through contract PN 42N/2023-23140201.*

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IDENTIFICATION OF THE DEPENDENCE BETWEEN THE SHAPE OF ELECTRODES FOR PROCESSING METAL SURFACES THROUGH ELECTRIC DISCHARGES AND THEIR WEAR

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Keywords: graphite, electrodes, surface treatment, shape of electrode

Introduction: In order to improve the adhesion characteristics of insulation made of polymeric materials on metal surfaces with the help of composite materials with adhesive properties, it is necessary for the metal surface on which the insulation is to be deposited to be subjected to physical-chemical treatments. These treatments are either the action of some corrosive chemical agents that have an action controlled by a series of technological parameters such as its concentration, by electrochemical processes or by physical processes [1]. The latter can be of the CORONA type electric discharges, electric impulse discharges
Materials and methods: The procedure is carried out with the help of electrodes. As a result of these treatments, a series of polar groups as the type -NO_2 -CO_3 CO, appear which increase the polarity of the metal surface and maximize its compatibility with the adhesive composite material. This paper intends to present the dependence between the shape of the electrodes with which the treatment is performed and the quality of this treatment. The identification of these dependencies is necessary because after use the active end of the electrode changes its shape and size as a result of their consumption [2]. Following the change in the shape and size of the active part of the electrode, the treatment effect of the metal surface may suffer. The experiments have determined the maximum number of electric discharges at certain parameters that an electrode can withstand so that the loss of shape and size does not affect the quality of the superficial treatment [3].

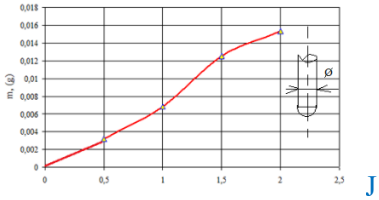

Fig. 1 Dependence of the wear of the "tool-electrode" with the shape of a hemisphere

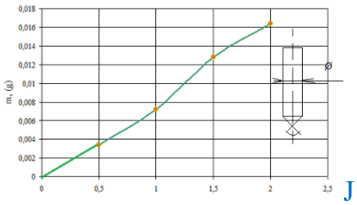

Fig. 1 Dependence of the wear of the "tool-electrode" with the shape of a hemisphere

Results: After performing surface treatments applied by electric discharges to the electrodes, the wear of the electrodes is directly proportional to the energy applied to carry out the electric discharges.
Conclusions: the wear of the electrodes, although somewhat more pronounced in the case of electrodes with a sharp tip, is insignificant until the application of energies of max 2.5 J. the treatment process is not affected in this way.

***Acknowledgements**: List funding sources in compliance to funder's requirements.*

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Synthesis, Antibacterial, Antioxidant and ADME Studies of Some Pyrimidine Compounds

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Introduction: Pyrimidine derivatives are of great interest because many have biological activities and clinical applications: nifedipine-type calcium channel blockers, antitumor, antibacterial, antiviral, anti-inflammatory, analgesic, anti-Alzheimer, antioxidant [1, 2].

Materials and methods: The pyrimidine compounds were synthesized by the Biginelli reaction and were characterized by 1H, 13C and two-dimensional NMR spectra. The aim of this study is to determine the antibacterial and antioxidant activities of some pyrimidine derivatives. To determine the antimicrobial activity of the synthesized compounds, the Kirby-Bauer diffusimetric antibiogram method was adapted. The antibacterial effect of pyrimidinone compounds against species representative of the main groups of pathogenic bacteria: Staphylococcus aureus ATCC 25923, Escherichia coli ATCC 25922 and Pseudomonas aeruginosa ATCC 27853 was evaluated. The antioxidant activity evaluated by the ABTS spectrophotometric method, and the results were reported in grams of chlorogenic acid equivalents (used as standard)/g compound. ADME study was performed using HyperChem program. All compounds had antibacterial effect against P. aeruginosa strain. E. coli was less sensitive to the action of pyrimidinone compounds, and S. aureus was resistant in the same context. The diffusimetric antibiogram (cylinder-plate technique) showed the largest diffusion area for the 3-hydroxy-substituted pyrimidine 3.

Results and conclusions: It was found that the presence of electron-donating substituents on the molecules and their positions on the benzene nucleus strongly influence the antimicrobial activity [3,4]. Summing up all the data obtained for the evaluated pyrimidinones, we conclude that the most promising compound to be used as an antimicrobial and antioxidant agent and with a good cell viability, is compound 3.

Acknowledgements: *This work was supported by the sectoral research-development plan (PSCD) project of the Ministry of National Defense „Innovative pharmaceutical preparations with topical administration and antimicrobial activity based on new synthetic hybrid compounds".*

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ADVANCED HYBRID MATERIALS BASED ON NATURAL POLYMERS: A NEW REMEDIATION STRATEGY FOR WATER CONTAMINATED WITH HEAVY METALS

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Keywords: chitosan, alginate, heavy metals, water remediation

Introduction: The current trend in the field of wastewater treatment is to develop the most effective methods for heavy metal removal. Of these, one of the most studied techniques is adsorption using adsorbent materials. Of these, one of the most studied techniques is adsorption using adsorbent materials [1]. Of these, one of the most studied techniques is adsorption using adsorbent materials. Adsorption is a technique that allows flexibility during design and implementation and in most cases is a high-quality effluent treatment [1-3]. The main challenges, at present, concern the creation of new adsorbent structures with increasing performance using cost-effective and environmentally friendly precursor materials and the implementation of sustainable and socio-economically viable technologies for the adsorption of heavy metals from wastewater or surface water. The main challenges, at present, concern the creation of new adsorbent structures with increasing performance using cheap and environmentally friendly precursor materials and the implementation of sustainable and socio-economically viable technologies for the adsorption of heavy metals from wastewater or surface water [2,3].

Materials and methods: The adsorbent materials produced during this research are based on a matrix based on natural polymers (such as chitosan and alginate) with a filler based on inorganic-organic composite which is obtained by host-guest polymerization. These materials were developed using a straightforward technique.

Results: Using X-Ray Diffraction (XRD), Fourier-Transform Infrared Spectroscopy (FTIR) and Scanning Electron Microscopy (SEM) the synthesis efficiency to produce new adsorbent materials was assessed from a physicochemical and morpho-structural point of view. Several adsorption models have been used to assess the materials' adsorption kinetics and determine their behavior during the adsorption process.

Conclusions: The developed adsorbents have promising applications in the efficient treatment of heavy metal charged water and are economically viable for large scale application.

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RELEASE KINETICS OF CURCUMIN FROM MICROBIAL POLYMERS BASED NANOSYSTEMS

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Keywords: nanosystems, microbial polymers, curcumin, release kinetics

Introduction: Curcumin, a polyphenol derived from *Curcuma longa, has* shown promising results in various diseases: cardiovascular, cancer, inflamations, infections, etc. However, curcumin has drawbacks like low water solubility, poor absorption, rapid metabolism, and quick systemic elimination which limit its therapeutic applicability. A solution to overcome these drawbacks is the encapsulation of curcumin in nanosystems [1, 2]. The release behaviour is very important in biomedical applications. The aim of this paper was to investigate the kinetic release of curcumin from nanosystems based on microbial polymers loaded with curcumin.

Materials and methods: Curcumin-loaded nanosystems with good entrapment efficiency (> 70%), nanometric size below 300 nm and narrow polydispersity index were obtained by nanoprecipitation method. The release kinetics of curcumin from nanosystems based on microbial polymers was determinated by a dialysis membrane method under sink conditions, at body temperature, under continuous stirring, using PBS 0.1 M pH 5 and PBS 0.1 M pH 7.4 as release media.

Results: *In vitro* release data from showed a biphasic profile characterized by an initial "burst effect" followed by a slower release reaching a maximum after 72 h. It was obseved a higher release rate of curcumin in neutral medium (pH 7.4) than in slightly acidic medium (pH 5). Several kinetics models such as Zero-order, First-order, Korsmeyer-Peppas, Higuchi and Hixson-Crowell were applied to predict curcumin release profiles from nanosystems based on microbial polymers. The release was best described by the Korsmeyer-Peppasand Higuchi models model indicating a Fickian diffusion mechanism.

Conclusions: The present study has shown that nanosystems based on microbial polymers can be used succsefully in various biomedical applications that implies a controlled release of active substances.

Acknowledgements: *This work was supported through the "Nucleu" Program, Contract no. 1N/2023, Project code PN 23-28 carried out with the support of MCID, project no. PN 23-28 03 01.*

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DESIGN AND ANALYSIS OF AN INNOVATIVE ENZYMATIC-FILTER (E.F) FOR PURIFYING AIR CONTAMINATED WITH SULFUR DIOXIDE (SO_2)

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Keywords: sulfur dioxide, oxidase, oxidation, purification system, clean air

Introduction: The project aims to provide a detailed overview of the installation to better optimize the processes of air purification from sulfur dioxide, as well as to offer a relatively affordable and fast method of air purification (using the oxidative abilities of enzymes).

Materials and methods: Basic reactions: Oxidation of hydroquinone to 1,4-benzoquinone: the enzyme oxidase, obtained from potatoes, catalyzes the oxidation of hydroquinone ($C_6H_4(OH)_2$) to 1,4-benzoquinone($C_6H_4O_2$). This process also involves interaction with molecular oxygen (O_2), which forms water (H_2O) as a by-product: $C_6H_4(OH)_2+O_2=C_6H_4O_2+H_2O$. Formation of sulfurous acid: in an aqueous environment, sulfur dioxide partially dissolves and hydrates, forming sulfurous acid (H_2SO_3). Reduction of 1,4-benzoquinone to 1,4-hydroquinone: benzoquinone reacts with sulfurous acid, taking two electrons and two protons, which leads to the formation of 1,4-hydroquinone: $C_6H_4O_2+2H^++2E^-=C_6H_4(OH)_2$. Oxidation of SO_2 to sulfuric acid: during the reduction of benzoquinone, sulfur dioxide is oxidized. This can occur through subsequent stages, with the formation of intermediates such as hydrosulfite and sulfite, but the final product of SO_2 oxidation will be sulfuric acid: $H_2SO_3+[O]=H_2SO_4$.

Conclusion: The data obtained make it possible to effectively apply this technique to purify the air from hydrogen sulfide in residential buildings, educational institutions, hospitals, as well as in industry. An operating hydrogen sulfide air purification system has been created, characterized by low energy consumption. The catalyst is not dangerous to the environment and humans, the process proceeds quickly at normal temperatures and pressures.

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WEARABLE MULTISENSING PATCH BASED ON SWCNT-PtNPs NANOCOMPOSITE FOR CLINICAL BIOMARKERS MONITORING FROM SWEAT

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Keywords: multisensing, wearable patch, biomarkers, sweat

Introduction: The application of nanotechnology and nanomaterials in (bio)electronics and biosensing tools production led to an extensive range of applications, allowing miniaturization and enabling their integration in many other devices[1]. Integration of nanostructured sensitive materials, based on carbon nanotubes and metallic nanoparticles equipped with stable enzymes selective layers into a wearable multisensing patch allowed a real-time monitoring of biological and physiological parameters (glucose, lactate, H_2O_2, pH etc) of individuals with high sensitivity and specificity compared to existing materials.

Materials and methods: Multisensing based biosensors were developed by functionalization of screen-printed carbon multi-working electrodes (SPE) with nanocomposites based on single-walled carbon nanotubes (SWCNT) and platinum nanoparticles (PtNP). Chitosan (CS) and sol-gel (SG) were used as immobilization matrices for bioreceptors, glucose (GOx) and lactate (LOx) oxidases, in order to achieve a high sensitivity and stability of the resulted biosensors for the clinical biomarkers (glucose and lactate). One of the working electrodes was functionalized only with SWCNT-PtNP for hydrogen peroxide detection.

Results: Electrochemical studies carried out with SWCNT-PtNPs/SPEs based sensors highlighted the enhanced electrocatalytic activity of the nanomaterial towards H_2O_2 reduction. The multisensing tool operated at a low applied potential of -0.2 V vs Ag/AgCl, displayed a specific sensitivity of 277.3 $mA \cdot M^{-1} \cdot cm^{-2}$, within a linear range of 0.037−21.5 mM, and a detection limit of 11.7 µM. The structural properties and enhanced electric conductivity of the SWCNT-PtNP based biosensors allowed a selective determination of glucose and lactate, with specific sensitivities of 168.04 and 128.58 $mA \cdot M^{-1} \cdot cm^{-2}$ for glucose and lactate, respectively. The applied potential was -0.05 V vs Ag/AgCl and the detection limits were 4.5 and 13.5 µM, within an extended linear range up to 2.2 mM. A wearable patch integrating the multisensing biosensor connected to a portable miniaturized potentiostate allowed the detection of glucose and lactate in sweat samples with good results.

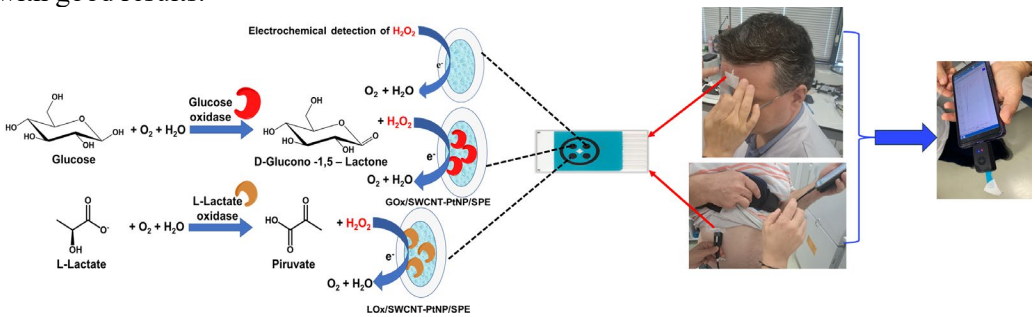

Figure 1. Multisensing of clinical biomarkers using portable biosensors.

Conclusions: The developed multisensing based biosensor facilitated the monitoring of various clinical biomarkers, such as glucose, lactate and H_2O_2, from biological samples, with increased stability, sensitivity and selectivity, being easily integrated in a miniaturized wearable patch.

Acknowledgements*: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project M-ERANET-3-FULSENS-GEL, Contract no. 318/2022 and by Core Program PN 23.06.01.01.*

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Marble degradation assessment via salt crystallization method

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Keywords: marble, salt crystallization, degradation

Introduction: Marble is an attractive natural stone, used for various application for both interior and exterior decorations for buildings. Due to its properties, it was used since ancient times and its use today is on a world-wide scale. However, when exposed to various exterior factors such as the soluble salts originated from the ground, street, atmosphere, jointing materials and backing materials, the salts can become entrapped in the pores of the marble and during day-night cycles or summer-winter can suffer a dissolution-recrystallization-hydration and the subsequent expansion can form microcracks and micropores that can grow and accelerate the material degradation [1-2]. The aim of this paper we will study the effect of salt on different types of marble (Ruschita marble, Albesti marble and Black marble).

Materials and methods: The sample were obtained by cutting pieces of marble with a diamond blade at the size of 40x40x15mm**.** The chemical weathering effect of salt crystallization on these stones was measured by exposing the samples to Na_2SO_4 x $10H_2O$ solutions (5, 12, 25% w%). by total immersion for 14 days at room temperature (about 20 °C). After immersion the test cubes were removed from the solution and dried in an oven for 24 h until they reached constant weight at 60°C and then cooled to room temperature. For this purpose, the dry weight loss test was conducted. The effects of salt crystallization have been observed by visual observations of damage patterns such as crack and deformation, detachment, and progressive loss of surface material through release of individual grains, rounded cube edges and granular disintegration.

Results: According to the results obtained the effect of salt crystallization is different: the most affected by the salt attack is Albesti marble where mass differences were observed (0,03; 0,04) and the most resistant is black marble where mass differences were observed (0.002=0.015).

Conclusions: Based on these results obtained we can conclude that loss of mass during salt crystallization artificial ageing tests: 25% Na_2SO_4 solution had the most destructive effects, whereas the 5% Na_2SO_4 solution was the mildest.

Acknowledgements*: This work was carried out through the PN 23.06 Core Program - ChemNewDeal within the National Plan for Research, Development, and Innovation 2022-2027, developed with the support of Ministry of Research, Innovation, and Digitization, project no. PN 23.06.02.01 (InteGral).*

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SECTION 2 - Bioresources, biotechnologies and biorefining (Oral communications)

1. *EDIBLE FOOD PACKAGING FROM YEAST BIOMASS FUNCTIONALISED WITH ESSENTIAL OILS*
2. *CONVERSION OF WASTE PLASTICS TO FUELS THROUGH PYROLYSIS*
3. *GEMMOTHERAPY - A HOLISTIC REVIEW*
4. *VALORIZATION OF TOMATO BY-PRODUCTS AND DEVELOPMENT OF A SUSTAINABLE GLUTEN-FREE PRODUCT*

EDIBLE FOOD PACKAGING FROM YEAST BIOMASS FUNCTIONALISED WITH ESSENTIAL OILS

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Keywords: edible films, biodegradable food packaging, food safety, yeast application, sustainability

Introduction: The growing interest towards sustainable food packaging replacing the existing petroleum-based ones triggered the development of innovative applications. Edible films and coatings are such examples of sustainable food packaging, based on proteins, carbohydrates, lipids or their combinations [1]. Among the major advantages of bio-based food packaging are: the ability to be functionalized with antioxidants, antimicrobials or probiotics, the biodegradability and cost-efficiency traits plus sustainability next to their renewability and low environmental print [2]. Yeast represents a low- cost, highly-available secondary product from brewing industry or from precision fermentation (i.e. genetically modified yeast for non-bovine casein production), which can be easily transformed into edible films due to its high protein content and polysaccharides. In line with the current effort for obtaining innovative biopolymeric materials, yeast biomass was used in this study to cast edible films [3] intended for food contact material use, functionalized with antimicrobial compounds from a mixture of cinnamon and lavender essential oils. The technology of yeast film formulation was optimized, and the casted films were characterized by physical, chemical and mechanical analysis.

Materials and methods: Yeast biomass (Belbake) was used to prepare 15% (w/w) solution which was denatured by sonication for 80 min, followed by thermal crosslinking at 80 ± 0.5 °C for 35 min. Glycerol and Tween 80 (1.00, 1.25, 1.50% w/w each) (Sigma Aldrich, USA) were added to the mixture for improving plasticity and surfactant properties in films. *Lavendula officinalis* essential oil (Lumea lavandei, Galati, Romania) and *Cinnamomum zeylanicum* essential oil (AromaZone, France) were used for functionalizing the film forming solutions. Small amplitude oscillatory shear and frequency sweeps, rotational steeped flow and peak hold measurements were performed on the film forming solution [1]. The dried films were stored at constant RH (30%), 20 °C until further testing for water activity by dew point mirror, mechanical properties by tensile testing, difference in color and transparency, film homogeneity by scanning electron microscopy, volatile fingerprint of the films analyzed by GC/MS, antimicrobial efficiency by disc diffusion assay and film digestibility [4].

Results: Rheological evaluation of the film forming solution indicated that all samples presented a shear-thinning behavior while the apparent shear viscosity ($3.1 – 3.3 \cdot 10^{-3}$ Pa·s) was not significantly influenced by the increasing content of glycerol and Tween at 100 s^{-1} shear rate. Flexible, resistant and homogenous yeast films with thickness of 0.19-0.30 mm, water activity ranging between 0.645- 0.659 and transparency of 47.48- 51.99% were obtained by casting (Figure 1). The lowest concentrations of glycerol and Tween, of 1.00% (w/v), contributed to the casting of the most transparent film. All films exhibited differences in color easily perceivable by consumers when compared to the corresponding control samples, without colored cinnamon EO. The SEM analysis indicated homogenous top-view surface of yeast films, while the film cross-section displayed disrupted yeast cells (Figure 2) resulted from the denaturation treatment.

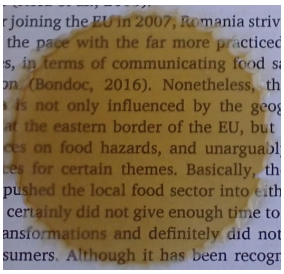
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Figure 1. Yeast biomass film

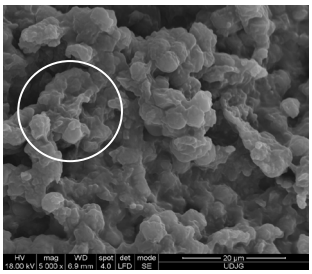

Figure 2. SEM cross-section of yeast film

The film with 1.00% glycerol and Tween showed the highest tensile modulus among all the tested films, that was 6 times higher as compared with 1.50% glycerol and Tween, indicating that the addition of glycerol and Tween made the films less rigid. Tensile strength increased approx. 3- fold with decreasing glycerol and Tween content from 1.5% to 1.0% for the films functionalized with EOs.The volatile fingerprint (VF) of yeast films with lavender and cinnamon mixture indicated the presence of cinnamaldehyde (14% of total VF) with the highest concentration in the sample with 1.50% glycerol and Tween, while cinnamyl alcohol acetate (4.19%) and eugenol (14.86%) were found in the highest concentration in the film with 1.0% glycerol and Tween. Other major flavor compounds tentatively identified in all samples were caryophyllene, 3-carene and humulene.

The edible films exhibited the highest antimicrobial activity against *Rhodotorula glutinis* (27.14 ± 0.87 mm) and *Geotrichum expansum* (22.62 ± 0.19 mm) and 44% lower compared to *R. glutinis* against *Bacillus cereus* (15.11 ± 1.13 mm). The bioavailability of yeast protein was similar in all tested samples during the 2h simulated digestion.

Conclusions: Flexible, resistant and homogenous baker yeast films were obtained and characterized. Edible yeast film packaging with lowest experimental concentrations of glycerol and Tween (1% w/v) were more transparent, capable to better retain eugenol and cinnamyl alcohol acetate compounds in comparison with other samples and exhibited the highest tensile stiffness and strength compared to the ones with higher plasticizer concentration. The lavender and cinnamon mixture triggered in films moderate antibacterial effect against *B. cereus* and strong antimicrobial activity against *R. glutinis* and *G. candidum*.

Baker's yeast (1 kg) can be transformed into approx. 1 m^2 yeast film with an estimated cost of approx. 1€/ m^2.

***Acknowledgements**: The authors acknowledge Grant Research RF 2486/ 31.05.2024 Dunarea de Jos University of Galati, Romania for funding resources, BioaAliment-TehnIA Integrated Center for* Research*, Expertise and Technological Transfer in Food Industry and Center of Excellence for Polymer Processing for the infrastructure provided.*

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CONVERSION OF WASTE PLASTICS TO FUELS THROUGH PYROLYSIS

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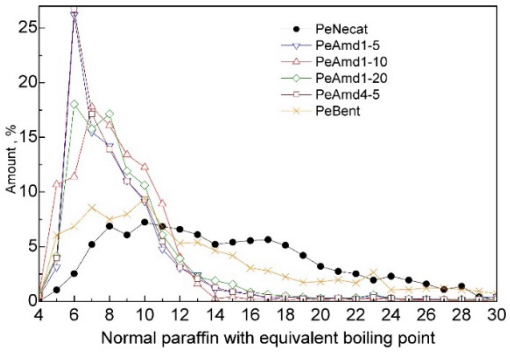
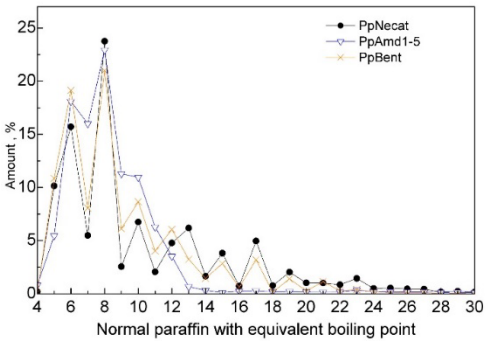
Keywords: polyethylene, polypropylene, pyrolysis, catalyst, fuels, waste

Introduction: In today's world, where plastic consumption and production are at an all-time high, understanding the chemical processes involved in their creation and breakdown is vital for sustainable resource management and environmental protection. One important process in this context is pyrolysis, a thermal decomposition method that can convert polymers like polyethylene and polypropylene into simpler compounds with a wide range of uses. In this paper will show the pyrolysis process using pure, then waste polyethylene and polypropylene with different calysts.

Materials and methods: *Experimental Setup:* A prototype laboratory setup used for the conversion of waste plastics into valuable fuels through pyrolysis; *Polymer Waste:* polyethylene (PE). Polypropylene (PP). The waste materials were sourced in the form of granules or film.

Results: The pyrolysis experiments conducted on polyethylene (PE) and polypropylene (PP) waste yielded distinct separation efficiencies for each polymer type. For PE, the separation efficiencies were: gaseous fraction (38.3%), naphtha (10.8%), diesel (15.9%), heavy paraffinic fraction (16.6%), and pyrolysis residue (18.3%). Similarly, for PP, the yields were: gaseous fraction (31.9%), naphtha (17.7%), diesel (17.1%), heavy paraffinic fraction (14.1%), and pyrolysis residue (19.2%). The analysis of the fractions revealed the presence of both saturated and unsaturated hydrocarbons, with iodine value testing confirming the existence of unsaturated compounds. This indicates that additional processing could be beneficial in improving the quality of the final products.





Conclusions: The described experimental setup and procedures enabled the effective conversion of waste plastics into valuable fuels via pyrolysis, offering important insights into the separation process and the characterization of the resulting products. The addition of catalysts in pyrolysis processes holds promise for enhancing the efficiency and quality of fuel production from waste plastics.

***Acknowledgements**: This work was carried out through the PN 23.06 Core Program - ChemNewDeal within the National Plan for Research, Development and Innovation 2022-2027, developed with the support of Ministry of Research, Innovation, and Digitization, project no. PN 23.06.01.01", AQUAMAT. Also, the authors acknowledge the support received from the Competitiveness Operational Program 2014-2020, Action: Stimulating the demand of companies for innovation through CDI projects carried out by companies individually or in partnership with CD institutes and universities, in order to innovate processes and products in economic sectors that show growth potential, MySMIS Code 122990, "INODES" financed by contract: 365/390041/27.09.2021.*

GEMMOTHERAPY - A HOLISTIC REVIEW

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Keywords: gemmotherapy, gemmoderivatives, holistic, protocols, homeopathy

Introduction: Gemmotherapy is a holistic therapy that uses plant embryonic tissues for health maintenance and restoration. Gemmotherapy for everyone is a concept of gemmotherapy, emphasizing its accessibility for general use. A brief history of gemmotherapy presents the origins and development of gemmotherapy, offering enough historical context for a general audience. Gemmotherapy identifying and responding to acute symptoms and their applications and effects.

Materials and methods: Gemmotherapy protocols for acute symptoms includes standardized protocols for about 40 conditions, such as fevers, exhaustion, spasmodic cough, and diarrhea. For example, the protocol for spasmodic cough involves two gemmoderivatives black currant (*Ribes nigrum*) and mountain cranberry (*Vaccinium vitis-idaea*). Black currant is said to reduce inflammation, support adrenal health, and enhance the effectiveness of other extracts, while mountain cranberry has a antiinflammatory, general tonic effect.

Results: Gemmotherapy involves using plant embryonic tissues (such as roots, buds, and shoots) in a specialized preparation that supports health by promoting drainage, detoxification, immune stimulation, and nutrition. These tissues are harvested and then macerated in a solution of alcohol and glycerin in a 1:20 ratio. After curing for three weeks, this mixture is filtered and further diluted in a 1:10 ratio before being bottled for sale. Despite some similarities with homeopathy, such as the dilution process and the use of D1 (or 1X) potency, gemmotherapy is distinct. The extracts are administered in a diluted form and are most effective when taken with at least four ounces of liquid (water, tea, or juice).

Conclusions: In terms of practical application, it is recommended that dosing extracts throughout the day by mixing the daily amount into a large water bottle, alternatively gemmotherapy extracts can be dropped directly making it adaptable to different lifestyles and age groups.

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Valorization of Tomato By-Products and Development of a Sustainable Gluten-Free Product

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Keywords: economic benefits, reduce waste, celiac consumers, innovative concept

Introduction: Utilizing residues from the agri-food industry brings both economic benefits and positive environmental impact. Given the impossibility of fully preventing residues, transforming food by-products into new products emerges as the main solution to reduce waste, accelerating the food sector's transition to a circular and sustainable economy.

Materials and methods: Considering the underutilized functional potential of vegetable by-products in the food industry, as well as the increased demand for gluten-free products in the global market, this study focuses on using residues from tomato processing as sustainable sources of antioxidants, carotenoids, and other natural pigments for developing sorghum flour-based crackers enriched with tomato waste powder, targeting both celiac and diabetic consumers. Laboratory tests have demonstrated the bioactive potential of tomato waste by determining the total content of carotenoids, lycopene, total polyphenols, and assessing antioxidant activity. The final product is based on an innovative concept, adding value to an improved gluten-free product both nutritionally and sensorially.

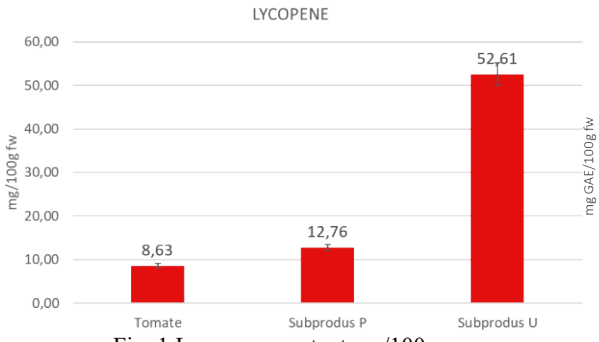

Fig. 1 Lycopene content mg/100g

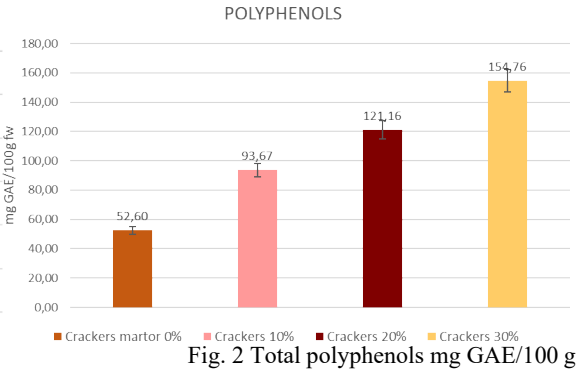

Fig. 2 Total polyphenols mg GAE/100 g

Conclusions: Tomato processing residues are sustainable sources of antioxidants, carotenoids (lycopene), and other natural pigments. Moreover, the final product is based on an innovative concept, adding value to a gluten- free product enhanced both nutritionally and sensorially, also fitting the "clean label" concept, suitable for all consumer categories Utilizing vegetable by-products contributes to a circular economy by minimizing pollution issues.

SECTION 2 - Bioresources, biotechnologies and biorefining (Poster presentations)

1. *DEVELOPMENT OF GC-MS/MS METHODS FOR THE SCREENING OF ORGANOCHLORINE AND ORGANOPHOSPHATE PESTICIDES IN COMPOST AND SOIL*
2. *PROCEDURE FOR THE RECOVERY OF VITICULTURAL WASTE FOR THE DEVELOPMENT OF NEW SPF COSMETIC FORMULATIONS*
3. *ASSESSING BIOFILM/BIOFILTER SYSTEMS EFFICIENCY FOR MUNICIPAL WASTEWATER TREATMENT*
4. *STUDIES REGARDING WATER RESOURCE POLLUTION WITH FERTILIZERS WHICH CONTAIN MICROBIAL BIOMASS*
5. *ANALYSIS OF MOLECULAR, QUANTUM AND BIOACTIVITY PROPERTIES OF SOME POLYPHENOLS COMPOUNDS OF GREAT THERAPEUTIC INTEREST*
6. *BIOCHAR BY PYROLYSIS OF SOLID DIGESTATE RESULTING FROM ANAEROBIC DIGESTION OF SPENT PLEUROTUS SUBSTRATE*
7. *BIOCHAR BY PYROLYSIS OF SOLID DIGESTATE RESULTING FROM ANAEROBIC DIGESTION OF SPENT PLEUROTUS SUBSTRATE*

DEVELOPMENT OF GC-MS/MS METHODS FOR THE SCREENING OF ORGANOCHLORINE AND ORGANOPHOSPHATE PESTICIDES IN COMPOST AND SOIL

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Keywords: GC-MS/MS, compost, soil, solid phase extraction, purification glass column

Introduction: Many chemicals pose significant environmental concern due to their detectable presence in various environmental components, toxicity, tendency for bioaccumulation, persistence, and potential for long-range transport. Among these are organochlorine [1] and organophosphate pesticides [2]. This study aimed to develop GC-MS/MS target analysis methods [3], to assess the levels of organochlorines (1,2,3,4,5,6-hexachlorocyclohexanes-HCH isomers, aldrin) and organophosphates (chlorpyrifos, chlorpyrifos-methyl) in soil and compost.

Materials and methods: To spike the target compounds, 35 mL of spiking mix solution in acetone was added to approximately 70 g of soil or compost [4]. Between 5 to 10 g of spiked soil and compost were extracted in triplicates for 24 hours using Soxhlet extraction with toluene. Prior to extraction, the solid samples were spiked with internal standards: hexachlorobenzene (HCB) solution for organochlorines and triphenyl phosphate (TPP) for organophosphates. After concentration, extract clean-up was performed using two approaches. First, SPE columns containing 500 mg silica (55 µm, 70 Å) were used with 3 x 3 mL of n-hexane. Second, glass columns packed with 4 g of silica gel deactivated with 10% water (w/w), topped with approximately a 1 cm layer of anhydrous Na_2SO_4, were employed. Target compounds were eluted with 60 mL of hexane. Prior to GC-MS/MS analysis, a recovery standard (RS) consisting of heptachlor was added. An Agilent 7890B Gas Chromatograph (GC) coupled to Agilent 7010 triple quadrupole mass spectrometer (Agilent Technology, Palo Alto, USA) operated in multiple reaction monitoring (MRM) mode was employed for the quantification of target compounds. Target pesticides were separated on an Agilent HP-5MS capillary column under the following temperature program: initial 40 °C (5 min isothermal), ramp with 5 °C min^{-1} to 110 °C (0 min), 20 °C min^{-1} to 180 °C (0 min), 5 °C min^{-1} to 230 °C (0 min) and 20 °C min^{-1} to 310 °C (3 min stationary).

Results: The measured concentrations were ranged between 0.03 µg/g for chlorpyrifos and chlorpyrifos-methyl in soil samples, and 0.19 µg/g for γ-HCH in compost samples, showing the advantages of the MRM method used. The concentration assessment indicated good recoveries for several compounds. Aldrin showed recoveries of 116.21 % in soil and 117.29 % in compost, α-HCH had 77.85 % in soil and 73.79 % in compost, β-HCH yielded 74.39 % in soil and 81.00 % in compost, while δ-HCH had 103.18 % in soil and 63.45 % in compost. However, for other compounds, further optimization of the methodology is needed to ensure acceptable recoveries.

Conclusions: An efficient GC-MS/MS method was developed for assessing levels of organochlorine and organophosphate pesticides in soil and compost. This study clearly demonstrated the ability to analysis a wide range of compounds in complex soil and compost matrixes.

***Acknowledgements**: This research was performed within the project PNRR-III-C9-2022-I9, contract no. 760265/06.03.2024, entitled "New Paradigms in Compound Specific Isotope Analysis for Assessment of Environmental Fate of Emerging Contaminants" – CF34/19.12.2023 ("Postdoctoral Fellowships") funded by Ministry of Research, Innovation and Digitalization (MCID), through Romania's National Recovery and Resilience Plan (PNRR).*

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PROCEDURE FOR THE RECOVERY OF VITICULTURAL WASTE FOR THE DEVELOPMENT OF NEW SPF COSMETIC FORMULATIONS

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Keywords: plants, waste, extracts, metallic nanoparticles, cosmetic formulations

Introduction: The wine sector, an essential component of the agri-food industry, represents one of the largest and most complex industries worldwide. It is recognized that inefficient waste management can lead to significant environmental problems. At the same time, the viticultural and wine waste have a low economic value and limited applications. However, current scientific studies indicate that these wastes are rich in bioactive compounds, thus highlighting their possibilities of use in various sectors. This research aimed to establish a technique for repurposing viticultural waste by formulating innovative SPF cosmetic formulations that integrates nanomaterials alongside natural extracts.
Materials and methods: The process of acquiring natural extracts from viticultural by-products involved the application and optimization of temperature classical extraction, and a modern microwave-assisted extraction, to yield extracts that are abundant in phytoconstituents. Further characterization of the extracts was conducted through the application of the spectrophotometric method using the Folin-Ciocâlteu reagent, alongside the High-Performance Liquid Chromatography (HPLC) technique. The extracts were used to synthesize monometallic and bimetallic nanoparticles by means of green chemistry. The nanomaterials were characterized by different analytical methods: UV-Vis spectroscopy, X-ray diffraction (XRD), X-ray fluorescence (XRF) and transmission electron microscopy (TEM). The bioactive properties of the nanoparticles were determined by evaluating their antioxidant and antimicrobial activity. The extracts and nanoparticles that were developed were further used as active ingredients in the formulation of gels and lip balms designed to provide sun protection factor.
Results: The applied characterization methods validated the ecological and rapid synthesis (3 hours) of mono and bimetallic nanoparticles, having small dimensions, with a spherical shape and a uniform dispersion in solution, emphasizing the presence of a core-shell type structure in the case of bimetallic nanostructures. Formulations of gels featuring a moderate SPF level, along with lip balms exhibiting SPF values ranging from 34 to 107 (Figure 1), have been created.

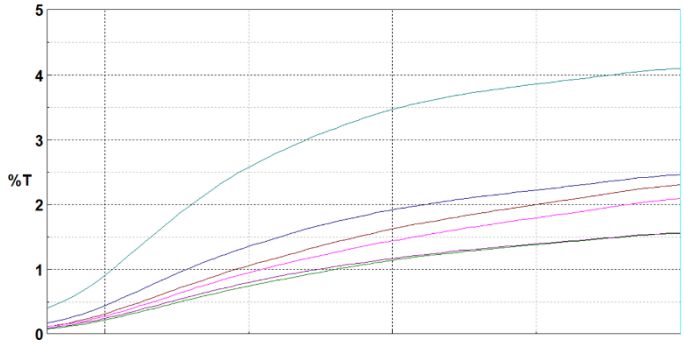

Figure 1. UV transmittance spectra for lip balm samples

Conclusions: The studies have demonstrated that by-products from viticultural and winemaking can be utilized as a valuable resource in the formulation of novel cosmetic products that offer sun protection.

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ASSESSING BIOFILM/BIOFILTER SYSTEMS EFFICIENCY FOR MUNICIPAL WASTEWATER TREATMENT

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Keywords: Pseudomonas aeruginosa, wastewater treatment, biofilm-biofilter systems, biotreatment

Introduction: With the increasing pressure on freshwater resources, the need to find efficient and sustainable solutions for wastewater treatment is becoming more urgent. In this context, the use of sustainable and promising alternatives to traditional methods, such as bacterial biofilm/biofilter systems, offers numerous benefits both for the environment and from an economic perspective. In this study, laboratory-scale experiments were conducted to evaluate the efficiency in reducing or eliminating various contaminants present in synthetic municipal wastewater by using a bacterial strain of *Pseudomonas aeruginosa*, employing different types of biofilters (i.e., commercially available solid supports) for bacterial biofilm formation.
Materials and methods: Microorganisms: *Pseudomonas aeruginosa* ATCC 27853; Biofilters: biofilters made of polypropylene, polyethylene and acrylo-butadiene styrene/polypropylene. Synthetic wastewater obtained according to [1]. The removal efficiency of contaminants such as organic compounds and nutrients [NO_3^- (nitrates), NO_2^- (nitrites), NH_4^+ (ammonium), PO_4^{3-} (phosphates), and SO_4^{2-} (sulfates) ions] were evaluated through COD (Chemical Oxygen Demand) and spectrophotometric analyses, respectively.
Results: The experimental results demonstrated the high capacity of the *Pseudomonas aeeruginosa* strain to reduce contaminants in wastewater, with the process being more efficient in the presence of solid supports. The study achieved notable reduction efficiencies across various water quality parameters, demonstrating the effectiveness of the treatment process. COD, which is an indicator of organic pollutants, was reduced by up to 68%, indicating significant improvement in organic matter removal. Additionally, nitrate and nitrite ions were reduced by 78%, and 93%, respectively, highlighting the potential of biofilm/biofilter systems for mitigating toxic and eutrophication nitrogen compounds. Ammonium ion levels were cut by 50%, while phosphate and sulfate ions were reduced by 52% and 44%, respectively, showcasing balanced performance in controlling both nutrient and inorganic pollutant levels.
Conclusions: These results have significant practical importance, as the bacterial strain used is commonly found in wastewater, meaning the treatment process can be carried out without the need for additional bacterial inoculation, but simply by introducing solid supports for biofilm formation. Another aspect to consider is that the treatment process occurs with low energy consumption, resulting from the use of a reduced aeration period.

***Acknowledgements**: The financial support was provided by Ministry of Research, Innovation and Digitization, through contract PN 42N/2023-23140201.*

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STUDIES REGARDING WATER RESOURCE POLLUTION WITH FERTILIZERS WHICH CONTAIN MICROBIAL BIOMASS

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Introduction: To effectively utilize the solid by-products resulting from industrial biosyntheses, one potential approach is to use them as fertilizers for agricultural soils or as components for developing new fertilizer formulations. In this regard, this research study aimed to assess the impact of two different types of fertilizers derived from spent microbial biomass on water quality, particularly regarding the potential loss of nutrients through leaching from rainwater [1-4].
Materials and methods: The experimental investigations were conducted using laboratory-scale glass columns filled with a mixture of red-brown soil, sand, and the respective fertilizers. The application rates respect the standard fertilization norms for Romanian soil. Each experimental variant simulated a specific average rainfall rate. After that, the nutrient losses resulting from leaching were quantified.
Results: The observed similarity in the behavior of fertilizers formulated with microbial biomass and complex fertilizers led to the conclusion that the impact on water quality from using fertilizers with microbial biomass is minimal.

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ANALYSIS OF MOLECULAR, QUANTUM AND BIOACTIVITY PROPERTIES OF SOME POLYPHENOLS COMPOUNDS OF GREAT THERAPEUTIC INTEREST

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Keywords: quantum reactivity descriptors, DFT computations, bioavailability, polyphenols

Introduction: The benzene nucleus and its derivatives (hydroxyl, carboxyl, methoxyl) are at the basis of so-called vegetal polyphenols, attributed with a plethora of pharmacological activities and also with various metabolic characteristics [1]. Resveratrol, phloretin and naringenin are examples of very active vegetal polyphenols whose bioavailability, formulation needs and bioactivity upon the eukaryotic cells can be estimated based on the in silico studies.

Materials and methods: Quantum mechanical calculations referring to molecular descriptors and chemical reactivity parameters for resveratrol, phloretin and naringenin were performed in gas phase using DFT/B3LYP/ 6-311 (d, p) density functional [2, 3] on the optimized geometries, after applying Merck molecular force field (MMFF) [4]. After setup of algorithm and basis set, computations on molecular properties and key structural descriptors were done. From predicted energies obtained for the frontier molecular orbitals (FMOs) - HOMO, and LUMO, respectively, a series of quantum parameters describing chemical reactivity and kinetic stability of these investigated structures, have been calculated: ΔE - FMOs energy gap I - ionization potential; A - electron affinity; η – chemical hardness; χ - electronegativity; μ - chemical potential; σ – chemical softness; ω - electrophilicity; ε – nucleophilicity. Additionally, to gain valuable information about specific targets binding, the bioactivity scores against six main cell modulators have been predicted: the G protein-coupled receptors (GPCRs), the ion channel, the kinase inhibitor, the nuclear receptor, the protease, and the enzyme inhibitor activities, respectively.

Results: In silico results pointed out the high stability and the ability of phloretin to pass the blood brain barrier (BBB); resveratrol and naringenin likely target the common oral-intestinal absorption in humans; phloretin and naringenin are also more likely to interfere with the activity six cell modulators connotative for the function of eukaryotes (e.g., G protein-coupled receptors (GPCRs), ion channel, kinase inhibitor, nuclear receptor, protease inhibitor and general enzyme inhibitor activity).

Conclusions: In silico data are very useful for the field of natural derived products by predicting important biophysical and biological properties and thus, achieving their maximum efficiency in humans, in the same time warning about the potential negative impact upon some other functions in human body.

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BIOCHAR BY PYROLYSIS OF SOLID DIGESTATE RESULTING FROM ANAEROBIC DIGESTION OF SPENT PLEUROTUS SUBSTRATE

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Keywords: biochar, solid digestate, pyrolysis

Introduction: The aim of this study is to obtain and characterize biochar samples resulting from the slow pyrolysis of solid digestate obtained from the comparative anaerobic digestion of Spent Pleurotus Substrate (SPS) and hay, both types of substrates with and without enzymatic pretreatment. Due to its' greater carbon content, porous surface, and a higher cation exchange capacity, biochar gained increasing interest towards recycling spent mushroom substrate through pyrolysis, and using the resulting biochar for the cultivation of a new mushroom generation. Other applications include removal of organic pollutants from wastewaters [1, 2].

Materials and methods: Samples from the lyophilized solid digestate were used to carry out the pyrolysis process, in a tubular reactor, under nitrogen atmosphere. The resulting fractions consist of biochar (solid), bio-oil (liquid) and pyrolysis gases. For each experiment, the 3 fractions were monitored to determine the mass balance, respectively product distribution. Biochar samples obtained from the pyrolysis reaction were characterized structurally and morphologically by SEM-EDS analysis using the Hitachi TM4000plus II scanning electron microscope, and BET analysis using NOVA 2200e Gas Sorption Analyzer (Quantachrome).

Results: From the SEM analysis of the biochar samples, the presence of acicular nanostructures can be observed, in the samples obtained by pyrolysis of the digestate from hay, both in samples with and without enzymatic pretreatment. On the other hand, in the case of the samples obtained by pyrolysis of the digestate from the processes using SPS as a substrate, a better homogeneity of the nanoparticles of smaller sizes is observed. The adsorption-desorption isotherm of the biochar obtained by pyrolysis of solid digestate resulting from the anaerobic digestion process of SPS are type II, presenting a hysteresis of type H3, meaning it does not present any adsorption limitation at a high-level p/p0. H3-type hysteresis is often encountered in mesoporous materials. In the case of biochar samples obtained by pyrolysis of digestate from hay, the results suggest that there is an irreversible adsorption of nitrogen inside the pores, the desorption curve being much higher than the adsorption curve. This may indicate that the nitrogen has been absorbed into pores that are not easily accessible or that there are small or restricted pores within the material.

Conclusions: The pyrolysis of SPS derived solid digestate, led to the production of biochar in larger amounts, significantly higher than the ratio of biochar obtained from hay derived biochar. On the other hand, there were no significant differences between enzymatically pretreated and non-treated samples. The preliminary observations obtained from SEM, are confirmed by BET analysis, where the average specific surface is higher in the case of SPS compared to hay. The difference in specific surface may also be due to the presence of pores with larger diameter and total volume in the case of SPS samples compared to hay.

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POTENTIAL OF SPENT PLEUROTUS SUBSTRATE FOR BIOMETHANE PRODUCTION

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Keywords: SPS, anaerobic digestion, pretreatment method

Introduction: The aim of this paper is to evaluate the performance of Spent Pleurotus Substrate (SPS) as feedstock in the anaerobic digestion process for biomethane production in comparison with the more traditional hay feedstock, and to determine the potential of enzymatic pretreatment to improve biodegradability and facilitate methanogenic processes. Given the rapidly increasing mushroom industry for human consumption, larger amounts of spent mushroom substrate is generated yearly which in the absence of proper waste management, can result in water and soil contamination. The typical handling of this type of waste includes incineration, landfilling and composting, which are harmful for the environment [1, 2].

Materials and methods: Using the equipment Gas Endeavour, five sets, each in triplicate were subjected to anaerobic digestion, samples consisting of control, SPS with and without pretreatment, hay with and without pretreatment. The chosen pretreatment option consisted of an enzymatic solution in which the dry samples were immersed prior to starting the anaerobic digestion process. Experiments were carried out for 25 days, with biomethane production being measured by the equipment's software throughout this period, but after day 16 no more signals were recorded for biomethane, indicating the end of the methanogenic process. At the end of the anaerobic digestion process, the samples were processed and analyzed to determine: dry matter; organic matter; chemical oxygen demand; volatile fatty acids; nitrogen, phosphorus and potassium content.

Results: Methane production showed that larger quantities were collected for hay samples, while the SPS samples plateaued at a lower methane production level within a shorter time. Including a pretreatment step led to partial consumption of hay substrate, which in turn led to a lower biomethane production, while in the case of SPS samples, biomethane production was improved, and the plateau was reached faster and was slightly higher. GC-MS analysis of dimethyl ether extract from liquid digestate, show that the primary volatile fatty acids in all samples are butanoic acid (13÷17% for hay, respectively 22÷24% for SPS) and hexanoic acid (47÷63% for hay, respectively 52÷60% for SPS), but the type of substrate used and the presence or absence of enzymatic pretreatment led to small variations in their distribution.

Conclusions: The volume of methane recorded the highest values using hay as a substrate. By including an enzyme pretreatment stage, both a decrease in the volume of methane produced and a delay in the initiation of the anaerobic digestion process were observed for hay samples. In the case of SPS biomass, the effect of the enzymatic pretreatment was positive, leading to a reduction in the time required to start the anaerobic digestion process, as well as a slight increase in the average volume of methane recorded in the triplicate samples. In the case of the control samples, consisting of the inoculum and distilled water, no signal was recorded in terms of volume of generated gas, suggesting that biomethane production can be attributed entirely to the digestion of the substrate used.

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ASSOCIATED EVENTS

1. *INCLUSIVE CO-CREATION FOR SUSTAINABLE RESEARCH IMPACT – INSPIRE*
2. *INNOVATION: MYSTERY OR A SYSTEMATIC APPROACH?*
3. *INTEGRATING STANDARDISATION, KNOWLEDGE VALORIZATION, AND SCIENCE DIPLOMACY*
4. *INTEGRATED APPROACH FOR WATER TREATMENT AND MONITORING – AQUAMAT PROJECT*
5. *NANOTECHNOLOGY-BASED DENTAL MATERIALS*
6. *RESEARCH ON THE DEVELOPMENT OF SUSTAINABLE TECHNOLOGIES FOR OBTAINING AND CAPITALIZING ON INNOVATIVE INGREDIENTS AND FOOD PRODUCTS, FOR THE NUTRITIONAL BALANCE OF THE MODERN CONSUMER'S DIET*
7. *NEW OXYGEN-CARRYING SYSTEMS BASED ON NANOCELLULOSE FOR WOUND HEALING*

INNOVATION: MYSTERY OR A SYSTEMATIC APPROACH?

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Moderators: Nicolae Varachiu, Bogdan Trica

A satellite event of **PRIOCHEM XX**, held on Oct. 15th, 2024, in hybrid format, brought together 33 participants (28 in meeting room at ICECHIM and 5 on-line), of which 11 are representatives of entities as companies, institutes, universities, organizations, and 22 are researchers from ICECHIM. In addition to the Romanian entities ICECHIM, ICI / Romanian National Competence Center in High Performance Computing (RONCC), SOFTWARE IMAGINATION & VISION – SIMAVI, Institute of Spatial Sciences, Cambus-Labs, PRIMPREST, UNST Politehnica Bucharest, Măgurele Science Park and KemaTronic-Baia Mare, participated also ECO-SISTEMI, a company from Italy and two multinational companies, VALENTA and VOGELSANG.

The moderator of the round table, Dr. Nicolae Varachiu, innovation manager, and the co-moderator, Dr. Bogdan Trică, senior researcher, both from ICECHIM, presented a "starter" and, further, guest representatives made short presentations too.

Discussions related to the knowledge and skills needed in the innovation process, presentations of best practices and exploration of future collaborations followed. Being a good example of a mystery for many people, but also of a systematic approach, for over 50 years, for specialists in the field, AI (Artificial Intelligence) was the center of attention. From presented examples and experience exchange, one important conclusion was that full attention should be paid when using AI, as quite similar inputs and requirements could provide different output answers by using an AI software; as for any software tool support, we could notice that still applies “garbage in, garbage out”, and still a human subject matter expert in the investigated field could help.

The participants appreciated as very useful the discussions, the exchange of knowledge, information, ideas for best practice and examples related to the innovation process; also related to application in present and especially in the future of AI in research and innovation, of available skills and resources from participants too, including software programs, and significant computing capabilities, with free access, available by RONCC.

Contacts have been established that will be exploited in the future through the continuation of collaborations and through establishing consortia, for participation in competitions, including from European funds. Even in the next weeks, ICECHIM and two SME companies, participants at round table, applied with the project "Industrial treatment plant, wastewater, CO2 recovery, hydrogen production and energy efficiency" at call for projects “Support for newly established innovative enterprises" through the Smart Growth, Digitization and Financial Instruments Program – POCIDIF, a program co-financed from the European Regional Development Fund (ERDF).

NANOTECHNOLOGY-BASED DENTAL MATERIALS

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Moderator: Radu Claudiu Fierascu

The workshop *"Nanotechnology-Based Dental Materials"* will showcase the transformative advancements achieved through the project *"Through Nanotechnology Towards the Next Generation Dental Restorative Materials,"* led by Dr. habil. Radu Claudiu Fierascu. This initiative represents a leap forward in the field of restorative dentistry, combining cutting-edge nanotechnology with biomaterials science to develop innovative dental solutions that address long-standing clinical challenges.

The project's primary accomplishment is the creation of a novel class of dental restorative materials characterized by simultaneous antibacterial activity and superior mechanical properties. This breakthrough was achieved through the strategic integration of substituted apatitic nanomaterials, functionalized with metallic nanoparticles, and natural bioactive compounds. These materials, designed for incorporation into cement-based systems such as glass-ionomer cements, demonstrate the potential to revolutionize dental restoration by enhancing both functionality and longevity.

Key highlights to be explored during the workshop include:

- **Synthesis and Functionalization:** Insights into the design and engineering of substituted apatitic nanomaterials, tailored for optimal bioactivity and mechanical resilience.
- **Nanotechnology Meets Nature:** The role of metallic nanoparticles and natural compounds in providing antibacterial protection and promoting tissue compatibility.
- **Performance Testing:** A comprehensive analysis of the mechanical strength, durability, and antibacterial efficacy of the developed materials in glass-ionomer cement applications.
- **Clinical Potential and Future Directions:** Discussion of the translational potential of these materials, bridging laboratory research with practical, patient-centered solutions in modern dentistry.

This workshop is a unique opportunity for researchers, dental professionals, and industry stakeholders to engage in discussions about the intersection of nanotechnology and restorative dentistry. Attendees will gain valuable insights into the project's findings, their implications for clinical practice, and the future of dental materials innovation. Join us as we unveil the next generation of dental restorative materials, redefining the standards of care and opening new frontiers in oral health.

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NEW OXYGEN-CARRYING SYSTEMS BASED ON NANOCELLULOSE FOR WOUND HEALING

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The project "Design of new nanocellulose-based gas-carrier systems" (CELGAS) addresses a topic of major interest in chronic wound healing in the aging population suffering from diabetes or obesity. The use of nanocellulose-based oxygen-carrying systems is a new solution in the treatment of chronic wounds that prevents wound infection and increases cell viability.

Oxygen-releasing biomaterials represent a new class of advanced materials developed for accelerating the healing process by avoiding inflammation and promoting angiogenesis [1-3]. Current oxygen delivery solutions have some limitations, such as pulmonary toxicity and limited oxygen diffusion for hyperbaric oxygen therapy, low oxygen carrying capacity of common oxygen carriers, and burst release of oxygen generating systems based on peroxides. Peroxidic materials used in oxygen-generating systems, such as calcium peroxide or magnesium peroxide, release hydroxyl radicals, which can be cytotoxic to cells in high concentrations. Moreover, excessive oxygen levels can induce oxidative damage to cells, while reactive oxygen species can alter cell differentiation. Therefore, the controlled release of oxygen by oxygen-releasing biomaterials is still a great challenge [1-3].

In this project, nanocellulose was used as a substrate for oxygen-generating materials. This choice was determined by the special properties of nanocellulose such as bio-degradability, non-toxicity, high specific surface area, good mechanical strength, availability of sources, and relatively low cost [4]. For a better control of oxygen delivery, nanocellulose was surface modified for increasing its reactivity or hydrophobicity by TEMPO-mediated oxidation, silane grafting, and grafting different naturally occurring organic acids or oligomers. The new oxygen-releasing biomaterials, which were developed in this project, are based on natural products with low toxicity. They may be obtained in the form of powder, injectable solution, or ointment and can be used in multiple therapies for healing cronic wounds and for treating bacterial and viral infections. The new solution schematically presented in the figure below can be easily scale-up for industrial production.

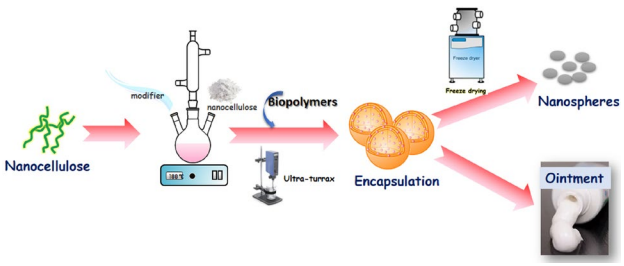

Figure 1. Schematic representation to obtain the new oxygen-releasing systems

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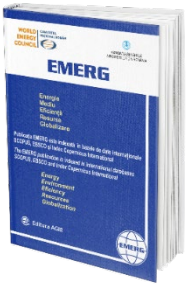

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