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BOOK OF ABSTRACTS

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Workshop
NEW MATERIALS FOR THE ELECTROCHEMICAL RECOGNITION OF INORGANIC AND BIOLOGICAL SPECIES
NOMARES 9

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IL1

DITHIOCARBOXYLATE ZWITTERIONS DERIVED FROM NHCs AND CAACs AND THEIR REDOX CHEMISTRY

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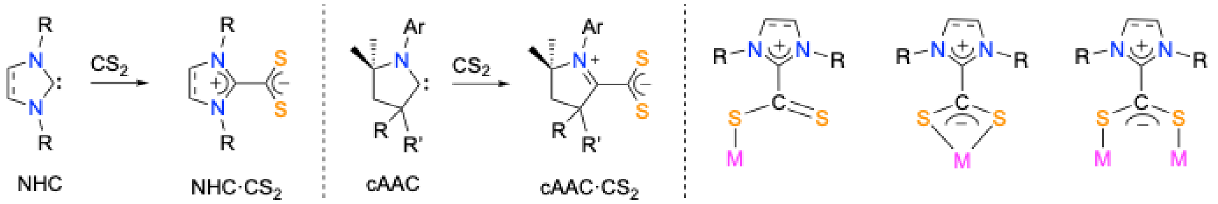
ABSTRACT

Since 2009,[1] our Laboratory has been investigating the synthesis, characterization, and coordination chemistry of dithiocarboxylate zwitterions derived from N-heterocyclic carbenes (NHCs) and cyclic (Alkyl)(Amino)Carbenes (cAACs).[2–7] These stable, crystalline inner salts form strong M–S bonds with a wide range of metal centers through various binding modes. As a result, they are particularly attractive for designing new molecular architectures based on transition metals, and we have already taken advantage of the resulting complexes for diverse biological and catalytic applications.



In this presentation, we shall disclose our latest results on the synthesis and complexation of NHC·CS$_2$ and cAAC·CS$_2$ zwitterions with a particular emphasis on their redox chemistry.

Keywords: azolium salts; carbenes; 1,1-dithiolate ligands; nitrogen heterocycles; ruthenium

References:

1. Delaude L., Sauvage X., Demonceau A., Wouters, J. Synthesis and Catalytic Evaluation of Ruthenium-Arene Complexes Generated Using Imidazol(in)ium-2-carboxylates and Dithiocarboxylates. Organometallics, 2009, 28, 4056–4064.

2. Mazars F., Hrubaru M., Tumanov N., Wouters J., Delaude L. Synthesis of Azolium-2-dithiocarboxylate Zwitterions Under Mild, Aerobic Conditions. Eur. J. Org. Chem. 2021, 2025–2033.
3. Zain Aldin M., Zaragoza G., Deschamps W., Tomani J.-C. D., Souopgui J., Delaude L. Synthesis, Characterization, and Biological Activity of Water-Soluble, Dual Anionic and Cationic Ruthenium-Arene Complexes Bearing Imidazol(in)ium-2-dithiocarboxylate Ligands. Inorg. Chem. 2021, 60, 16769–16781.
4. Touj N., Mazars F., Zaragoza G., Delaude L. Aldiminium and 1,2,3-Triazolium Dithiocarboxylate Zwitterions Derived from Cyclic (Alkyl)(Amino) and Mesoionic Carbenes. Beilstein J. Org. Chem. 2023, 19, 1947–1956.
5. Zain Aldin M., Zaragoza G., Choquenet E., Blampain G., Berger G., Delaude L. Synthesis, Characterization, and Biological Activity of Cationic Ruthenium-Arene Complexes with Sulfur Ligands. J. Biol. Inorg. Chem. 2024, 29, 441–454.
6. Carvalho V. P. Jr, Zaragoza G., Delaude L. Homoleptic Ruthenium(II) Complexes Bearing Imidazol(in)ium-2-dithiocarboxylate Ligands: Synthesis, Characterization, and Redox Properties. Dalton Trans. 2024, 53, 11436–11444.
7. Mazars F., Zaragoza G., Delaude L. Synthesis, Characterization, and Catalytic Evaluation of Ruthenium Complexes Bearing Xanthinium-8-dithiocarboxylate Ligands Derived from Caffeine and Theophylline. Organometallics 2024, 43, 2284–2304.

IL2

NANO-ENHANCED SYNTHETIC RECEPTORS: THE FUTURE OF ELECTROCHEMICAL DETECTION

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ABSTRACT

Molecular imprinting technology is a creative method that enables the creation of synthetic biorecognition sites that mimic natural biological entities such as antibodies, receptors, and enzymes. After the target analyte is removed, synthetic cavities enable the recognition and selective rebinding of the template. In this case, molecular imprinting technology offers biosimilar receptors with higher specific affinities and better stability than natural receptors and biomolecules [1]. Although stable and durable MIPs seem relatively easy to create for maximum efficiency, some optimization parameters should be considered, such as the appropriate functional monomer and crosslinker, as well as the optimal ratios of functional monomer, template, and crosslinker [2]. The optimization process can vary based on the polymerization technique. In addition, the structure of the polymeric matrices and the type of bond contact between the template and the polymer are two important factors in MIPs. It was reported that template monomer interactions occur via noncovalent forces, including van der Waals forces, hydrogen bonds, and dipolar interactions [1, 2]. Among them, MIP-based electrochemical sensors play a significant role because MIPs help overcome the lack of selectivity in electrochemical sensors. MIP-based electrochemical sensors and miniature electrochemical transducers can detect target analytes in situ. Thanks to their superior chemical and physical stability, low-cost manufacturing, high selectivity, and fast response, MIPs have recently become an area of active research. The increase in environmental awareness and stricter regulations for the use of chemicals and economic competitiveness are challenging the scientific community and industry to explore greener strategies in their processes, preventing pollution and reducing waste while maximizing the efficiency of the processes, and that can only be achieved by the application of green chemistry and engineering principles. Molecular imprinting has much to gain in applying these green tools since new alternative solvents and clean technologies, combined with computational tools, can optimize both the polymer and the process.

Keywords: MIP, functional monomer, polymerization, electrochemical sensors

References:

1. L. Uzun, A.P.F. Turner, Molecularly-imprinted polymer sensors: realising their potential, Biosens. Bioelectron. 76 (2016) 131e144.
2. S. Irem Kaya, Ahmet Cetinkaya, Sibel A. Ozkan, Trends in Environmental Analytical Chemistry, 37, (2023), e00193.

IL3

BIO-INSPIRED CARBOXYLATE-POLYMER/METAL OXIDES NANOCOMPOSITE AS EFFICIENT MATERIAL FOR ELECTROCATALYTIC WATER OXIDATION

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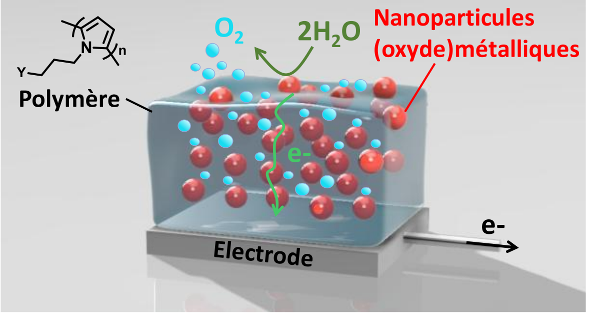
ABSTRACT

Water oxidation into dioxygen (OER) remains a critical bottleneck for scaling up water-splitting and CO_2-reduction electrolyzers due to its slow kinetics and high overpotential. The challenge lies in developing efficient, durable, and cost-effective OER catalysts using earth-abundant elements. Heterogeneous metal oxides or (oxy)hydroxides are the most promising candidates, balancing activity and robustness. Current research prioritizes oxides based on abundant metals like Co, Ni, Fe, Mn and Cu, cheaper alternatives to Ir and Ru oxides, that can be deposited as thin films on electrodes to create efficient anodes [1]. Nanostructuring is key to enhancing electrocatalytic performance, as is it increases the active surface area while reducing costs. Indeed, smaller particle sizes often compromise stability and can lead to aggregation. To adress this, immobilizing nanoparticles (NPs) within a polymeric or inorganic matrix has proven to be effective [2-5]. In this context, we recently developed bio-inspired nanocomposite electrode materials that are both highly active and stable for water oxidation, using a simple and versatile electrochemical method. These materials consist of nanosized, earth-abundant metal oxides ($M(M')O_x$, where M, M' = Ni, Co, Fe, etc.) uniformly dispersed in a polymer matrix with anionic functions [6]. This design mimics the carboxylate-rich environment and sub-nanosized structure of the natural Mn_4CaO_5 cluster of PSII, which are essential for exceptional catalytic efficiency. The method of elaboration of the nanocomposites, their characterization through complementary methods, and their electrocatalytic performance for OER will be presented.



Keywords: water oxidation; nanocomposite; metal oxides; polypyrrole

References:

1. Kanan, M. W; Nocera, D. G. Science 2008, 321, 1072-1075.
2. Shifrina, Z. B.; Matveeva, V. G.; Bronstein, L. M. Chem. Rev. 2020, 120, 1350-1396.
3. Morales, D. V.; Astudillo, C. N.; Lattach, Y.; Urbano, B. F.; Pereira, E.; Rivas, B. L.; Arnaud, J.; Putaux, J.-L.; Sirach, S.; Cobo, S.; Moutet, J.-C.; Collomb, M.-N.; Fortage, J. Catal. Sci. Technol. 2018, 8, 4030-4043
4. Morales, D. V.; Astudillo, C. N.; Anastasoaie, V.; Dautreppe, B.; Urbano, B. F.; Rivas, B. L.; Gondran, C.;

Aldakov, D.; Chovelon, B.; André, D.; Putaux, J.-L.; Lancelon-Pin, C.; Sirach, S.; Ungureanu, E.-M.; Costentin, C.; Collomb, M.-N.; Fortage, J. Sustainable Energy & Fuels 2021, 5, 4710-4723.
5. Collomb, M.-N.; Fortage, J.; Dautreppe, B.; Barré, R.; Leguerrier, D. M. d.. In L'actualité Chimique, Société Chimique de France: 2025; Vol. 504, pp 19-24
6. Dautreppe, B.; Fortage, J.; Collomb, M.-N. Électrode comprenant un revêtement composite et procédé de fabrication associé B04655 FR-A358-B2021-15 avril 2022.

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IL4

MODIFIED TITANIUM ELECTRODES BY HYDROXYAPATITE-BASED COATINGS FOR MEDICAL APPLICATIONS

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ABSTRACT

Orthopedic implants are expected to induce bonding with surrounding bone tissue, without causing harmful effects to the host body. Having in mind mechanical and load-bearing requirements that orthopedic implants have to endure, metals and metal alloys are a primary choice due to the excellent combination of stiffness, toughness, and strength. However, metallic implants are usually prone to corrosion, which in some cases can cause adverse effects on the host organism. Moreover, the lack of the osseointegration process when metallic implants are used limits their application. A promising approach for developing improved orthopedic implants could be applying thin bioactive films on the metal surface that would enhance implant bonding with damaged bone. Due to excellent mechanical properties and high corrosion resistance, titanium is often the metal of choice even though it lacks osseopromotive properties. Titanium surface modification by composite hydroxyapatite/chitosan/gentamicin coatings could overcome this problem, enhancing biocompatibility at the same time [1-3]. The electrophoretic deposition process (EPD) was used to obtain composite coatings with controlled topography and morphology at room temperature. Different physico-chemical (FTIR, SEM, XRD, HPLC), electrochemical (EIS, PDS) and biological (MTT cytotoxicity test, antibacterial activity test) coatings properties have been investigated. It was shown that deposited coatings are nontoxic against MRC-5 and L929 cell lines, and exhibit antibacterial activity against *Staphylococcus aureus* and *Escherichia coli* bacterial strains. Kinetics of gentamicin release in simulated body fluid at 37°C proved initial burst release favourable to quickly suppress the bacterial adhesion and biofilm formation. Based on obtained results the deposited hydroxyapatite/chitosan/gentamicin coatings on titanium can be considered for medical applications as hard tissue implants.

Keywords: titanium; hydroxyapatite; chitosan; gentamicin; electrodeposition

References:

1. M. Stevanović, M. Djošić, A. Janković, K. Nešović, V. Kojić, J. Stojanović, S. Grujić, I. Matić- Bujagić, K. Y. Rhee, V. Misković-Stanković, Assessing bioactivity of gentamicin preloaded hydroxyapatite/chitosan composite coating on titanium substrate, ACS Omega 2020, 5, 15433-15445.
2. M. Stevanović, M. Djošić, A. Janković, V. Kojić, J. Stojanović, S. Grujić, I. Matić- Bujagić, K. Y. Rhee, V. Misković-Stanković, The Chitosan-Based Bioactive Composite Coating on Titanium, J. Mater. Res. Technol. 2021, 15, 4461-4474.
3. V. Mišković-Stanković, T. Atanackovic, Novel Antibacterial Biomaterials for Medical Applications and Modeling of Drug Release Process, 1st ed.; Taylor & Francis/CRC Press: Boca Raton, USA, 2024, p.p.1-288.

OP1

ON EXPERIMENTAL AND CALCULATED PROPERTIES OF SEVERAL FORMAMIDINE DERIVATIVES

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ABSTRACT

Nitrogen-containing compounds such as amidines has been extensively studied owing to their importance as biologically active compounds. They have also found applications as monomers for polymer synthesis, bleaching agents for paper, ultraviolet light absorbers, and ligands in transition metal catalysis. In organic synthesis, formamidines serve as protecting groups for primary amines. They support linkers in solid-phase synthesis and auxiliaries in asymmetric synthesis. They also serve as building blocks for the synthesis of acyclic diaminocarbenes (ADCs) and N-heterocyclic carbenes (NHCs), especially those with six, seven and even eight membered rings [1]. In these applications, shape and H-bonding patterns are critical features that determine the resulting properties. *N,N´*-disubstituted formamidines derived from aryl and alkylamines have been well-characterized as *E*-isomers [2,3]. Formamidines **1** and **2** have been synthesized and characterized by elemental analysis, FT-IR, FT-Raman, ^{1}H and ^{13}C NMR spectroscopies and X-ray single crystal diffraction. The concentration-dependent spectral behavior of **1** and **2** were investigated in acetonitrile by UV–Vis spectroscopy. Electrochemical experiments were carried out by cyclic voltammetry, differential pulse voltammetry and rotating disk electrode voltammetry (CV, DPV, RDE) at several concentrations of **1** and **2** in acetonitrile in presence of tetrabutylammonium perchlorate as supporting electrolyte on glassy carbon electrode. The UV–Vis spectra showed a clear concentration-dependent increase in solutions absorbance, allowing the construction of linear calibration curves. This study provided a preliminary characterization of the new synthesised formamidines **1** and **2** through UV–Vis and electrochemical techniques. The DFT calculation were correlated with the experimental results. These results indicate that formamidines may be suitable for future optical or electrochemical applications.

Keywords: cyclic voltammetry, differential pulse voltammetry, formamidines, rotating disk electrode voltammetry, UV-Vis spectroscopy

References:

1. L. Rosen, V. M. Lynch, C. W. Bielawski, Organometallics 2010, 29, 3047–3053, doi: 10.1021/om1004226.
2. L. Xing, C. Wiegert, A. Petitjean, J. Org. Chem. 2009, 74, 9513–9516, doi: 10.1021/jo9020453.

3. M. J. U. Fink, C. Heiser, C. Wagner, K. Merzweiler, Z. Anorg. Allg. Chem. 2022, 648, e202200122, doi: 10.1002/zaac.202200122.

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OP2

ON THE ELECTROCHEMISTRY OF 2-((5-ISOPROPYL-3,8-DIMETHYLAZULEN-1-Y)DIAZENYL)-5-(5-ISOPROPYL-3,8-DIMETHYLAZULEN-1-YLTHIO)-1,3,4 THIADIAZOLE

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ABSTRACT

2-((5-isopropyl-3,8-dimethylazulen-1-y)diazenyl)-5-(5-isopropyl-3,8-dimethylazulen-1-ylthio)-1,3,4 thiadiazole (**L**) is a diazene derivative containing a thiadiazole heterocycle. This class of compounds is of interest due to its stability and its potential use in dyes, functional materials and redox-active systems. In this work, we investigated the UV–Vis and electrochemical properties of **L**, aiming to evaluate its redox behavior for potential optical and analytical applications[1]. The concentration-dependent spectral behavior of the azulene-based diazenes were investigated in acetonitrile by UV–Vis. The electrochemical experiments were carried out by cyclic voltammetry, differential pulse voltammetry and rotating disk electrode voltammetry (CV, DPV, RDE) at more concentrations of **L** in acetonitrile in presence of tetrabutylammonium perchlorate as supporting electrolyte (0.1 M TBAP, CH_3CN) on glassy carbon electrode. The UV–Vis spectra showed a clear concentration dependent increase in solutions absorbance, allowing the construction of linear calibration curves. **L** exhibits a characteristic absorption band in the visible region, consistent with the extended conjugation of the azulene unit. The CV study was performed on variable scan domains and at more scan rates. RDE studies were done at variable rotation rates. This study provided a preliminary characterization of **L** through UV–Vis and electrochemical techniques. These results suggest that L may be suitable for future optical or electrochemical applications.

Keywords: 2-((5-isopropyl-3,8-dimethylazulen-1-y)diazenyl)-5-(5-isopropyl-3,8-dimethylazulen-1-ylthio)-1,3,4 thiadiazole; UV-Vis; cyclic voltammetry; differential pulse voltammetry; rotating disk electrode voltammetry

References:

1. A.C. Razus, L. Birzan, M. Cristea, V. Tecuceanu, C. Draghici, A. Hanganu, M. Maganu, L. Pintilie and E.M. Ungureanu, New (azulen-1-yldiazenyl)-heteroaromatic Compounds Containing 1,2,5-thiadiazol-3-yl Moieties, Rev. Chim. (Bucharest) 2019, 70, 1518–1529.

Acknowledgment: This work was developed within the scope of the project Hybrid electrocatalytic procedures for the sustainable preparation of electrochemical sensors based on modified electrodes.

OP3

BISPHENOL A DETECTION USING MOLECULARLY IMPRINTED POLYMER BASED ELECTROCHEMICAL SENSOR

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ABSTRACT

The widespred use of synthetic polymers in food packaging and consumer products has led to increasing concern over the migration of hazardous chemical additives into the environment and human body. Among these compounds, bisphenol A (BPA) has attracted particular attention due to its frequent release from polymer-based materials under typical usage conditions. Even at low concentrations, BPA exposure has been associated with biological activity that may interfere with endocrine function, raising significant concerns regarding long-term health effects [1]. These risks highlight the urgent need for analytical techniques capable to detecting low concentration of BPA with reliability and precision. In recent years, electrochemical sensing platform have emerged as attractive alternatives to conventional analytical methods, offering advantages such as rapid response, portability and low operational cost. The integration of molecularly imprinted polymers (MIPs) into electrochemical sensors further enhances their performance by introducing highly selective recognition sites tailored to the target molecule [2]. Among conductive polymers, polypyrrole (PPy) stand out as a versatile candidate for MIP fabrication due to its excellent conductivity, facile electropolymerization and strong adhesion to electrode surfaces. In this study, a MIP-based electrochemical sensor for BPA detection was developed using gold screen printed electrodes (Au-SPEs) modified with sulfur-doped graphene to enhance the conductivity and surface area. Subsequently, PPy was electropolymerized in the presence of BPA as a template molecule to form the imprinted recognition layer. The electroplymerization parameters, including the applied potential and scan cycles were obtimized to improve the sensor performance. Additionally, the influence of different BPA concentrations on the imprinting efficiency was investigated, followed by optimization of the extraction process to ensure effective removal of the template and the formation of accessible binding sites and also optimization of BPA rebinding using incubation protocol for a certain period of time.

Keywords: bisphenol A; molecular imprinted polymer; sensor

References:

1. L.A. Dinu Gugoasa. Review—Electrochemical Sensors for Determination of the Endocrine Disruptor, Bisphenol A, J. Electrochem. Soc. 2020, 167, 037506.
2. Y. Li, L. Luo, Y. Kong, Y. Li, Q. Wang, M. Wang, Y. Li, A. Davenport, B. Li. Recent advances in molecularly imprinted polymer-based electrochemical sensors, Biosens. Bioelectron. 2024, 249.

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OP4

PHYTOCHEMICAL CHARACTERIZATION AND BIOLOGICAL ACTIVITIES OF EXTRACTS FROM AN ENDEMIC LAVENDER OF MOROCCO

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ABSTRACT

In the context of growing interest in natural alternatives to synthetic agents, the medicinal and aromatic plants endemic to Morocco are attracting particular attention due to their richness in bioactive compounds and their multiple potential applications. In this context, the present study aims to evaluate the phytochemical composition as well as the antioxidant, antifungal, and insecticidal properties of different extracts from an endemic Lavandula species from Morocco. The extracts were obtained using solvents of variable polarity (methanol, ethyl acetate and dichloromethane), allowing selective extraction of metabolites according to their physicochemical characteristics. Phytochemical analysis revealed that the methanolic fraction presents the highest contents in phenolic compounds (85.66 mg GAE/g) and flavonoids (8.50 mg QE/g), correlated with a marked antioxidant activity, evaluated by DPPH (IC_{50} = 13.26 µg/mL), FRAP (EC_{50} = 9.40 µg/mL) and total antioxidant capacity (228.05 mg AAE/g) tests. Furthermore, the dichloromethane extract showed moderate antifungal activity against Penicillium expansum (MIC ≥ 5 mg/mL), while the ethyl acetate extract distinguished itself by a significant insecticidal activity against adults of Tribolium castaneum (LD_{50} = 2.80 mg/cm²). These results highlight the potential of this plant as a source of bioactive metabolites with antioxidant and biopesticidal properties. They also underline the importance of scientific valorization of endemic species for their conservation and sustainable exploitation, thus contributing to the development of ecological solutions for crop protection and the production of natural antioxidants.

Keywords: endemic medicinal plant; phytochemical analysis; biological activities; valorization

OP5

SELF-REDUCED TIO$_2$ NANOTUBE ELECTRODE FOR METAL IONS DETECTION

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ABSTRACT

Electrochemical detection typically involves the deposition of metal ions onto the electrode surface either under open-circuit conditions (usually used with modified electrodes) or through controlled potential (usually used with solid electrodes). While the latter method improves selectivity, the former technique enables the simultaneous detection of multiple ions. When a semiconductor electrode is exposed to a particular wavelength while metal ions are present, simultaneous processes of metal ion accumulation and reduction occur at the electrode surface, resulting in an enhanced response of the electrode [1, 2]. Thus, new insights on heavy metal ion detection using self-reduced Ti/TiO$_2$ nanotube electrodes under photo-irradiation are being developed while taking prior considerations into account. Heavy metal ion detection is made possible by the synergy between photo-accumulation and sensing with these electrodes. Under photo-accumulation conditions, self-reduced TiO$_2$ nanotube semiconductor electrodes were employed for electrochemical metal ion detection in an open circuit. The electrodes surface characteristics caused them to react differently to metal ions at various light wavelengths. When exposed to light at 389 nm, the self-reducing electrode responded to Pb(II) and Cu(II) ions; at 426 nm, Hg(II) ions were detected in addition to Pb(II) and Cu(II) ions. At 389 nm, the detection limits for Pb(II) and Cu(II) using these electrodes 2×10^{-7} M and 8×10^{-9} M, respectively. The detection limits were 1×10^{-7} M, 3×10^{-9}, and 4×10^{-9} M for Pb(II), Cu(II), and Hg(II), respectively at 426 nm.

Keywords: self-reduced TiO$_2$ nanotube electrode; metal ions; photo-accumulation; electrochemical detection

References:

1. Buica, G.-O.; Stoian, A.B.; Manole, C.; Demetrescu, I.; Pirvu, C. Zr/ZrO2 nanotube electrode for detection of heavy metal ions. Electrochem. Commun. 2020, 110, 106614.
2. Pirvu, C.; Stanciu, G.; Buica, G.-O. Cu(II) and Hg(IIi) detection under photo-assisted accumulation in an open circuit potential at a polyazulene–EDTA like modified electrode. Analyst, 2022, 147, 4730–4734.

Acknowledgment: This work was supported by a grant from the National Program for Research of the National Association of Technical Universities—GNAC ARUT 2023.

OP6

TWO-DIMENSIONAL JANUS HfSSe AS A HIGH-PERFORMANCE ANODE MATERIAL FOR LI-ION BATTERIES: A DFT STUDY

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ABSTRACT

Regarding the alternative energy sources are being explored and developed as a result of the increased interest in renewable energy resources to complete the rising demands of our modern civilisation. The significant usage of digital devices has hastened the development of portable and lightweight batteries, which are crucial for renewable energy storage. The development of energy storage and electrochemical energy conversion technologies is therefore a major focus. Given this, two-dimensional (2D) materials have garnered significant interest, particularly concerning rechargeable batteries like lithium-ion batteries (LIBs). In this study, we employed first-principles calculations within the density functional theory (DFT) framework to examine the potential of 2D Janus transition metal dichalcogenide (TMD) Janus HfSSe, as anode materials for lithium-ion batteries. We explored the electronic properties before and after the adsorption of Li-ion on the Janus HfSSe monolayer. Additionally, we investigated the open circuit voltage and theoretical storage capacities of Li ions in the Janus HfSSe monolayer. Our results clearly show that the Janus HfSSe monolayer exhibits a substantial cohesive energy of –4.29 eV per atom, indicating excellent structural stability, and demonstrates semiconducting behavior characterized by an indirect bandgap of 0.91 eV. Based on energy and charge analysis, our findings reveal that the Se-bottom site is the most stable adsorption site for the Li atom on the Janus HfSSe monolayer, with a notable adsorption energy of –3.13 eV and substantial charge transfer of 0.88 e. Upon Li adsorption, the Janus HfSSe monolayer undergoes a phase transition from semiconductor to metal, which enhances its electrical conductivity and suitability as an anode material in LIBs. Furthermore, the calculated open-circuit voltage (OCV) ranges from 0.7 V as the Li concentration increases, indicating favorable electrochemical performance. And diffusion 0.2 eV at full lithiation, the Janus HfSSe monolayer achieves a remarkable theoretical storage capacity up to 555.5 $mAhg^{-1}$, significantly surpassing the capacity of many other monolayer materials. Overall, the findings of this work are expected to support the future design and improvement of rechargeable LIBs utilizing Janus HfSSe monolayers as a next-generation anode material.

Keywords: 2D materials, Anode, Janus HfSSe monolayer, Li-ion batteries

References:

1. M.S. Zyane, H. Rghioui, M. Ait Tamerd, A. Achahbar, M. Zanouni, A. Marjaoui, Mater. Today Commun. 108469 (2024).
2. H. Rghioui, M. Said Zyane, H. Ghannam, M. Ait Tamerd, M. Diani, M. Zanouni, and A. Marjaoui, Chem. Phys. Lett. 849, 141429 (2024).

OP7

COMPARATIVE INVESTIGATION OF ANTIOXIDANT POTENTIAL OF *PERILLA SPP.* EXTRACTS BY CHEMICAL AND ELECTROCHEMICAL ANALYSES

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ABSTRACT

Research into natural antioxidants has become increasingly important in various fields, such as medicine, health, or the food industry. Thus, in the search for new such antioxidant compounds, these properties are often investigated by several methods, for a more accurate validation. Most often, antioxidant activity is usually evaluated using various chemical tests by spectrophotometric methods, such as DPPH (free radical scavenging), ABTS (radical cation bleaching) or FRAP (ferric reducing power). Cyclic voltammetry is an electrochemical technique that can also provide complementary insights into antioxidant activity. This study explores the antioxidant potential of different extracts of *Perilla spp*. using both DPPH radical scavenging assay and electrochemical cyclic voltammetry. The extracts were obtained using classic and green solvents (NADES) and green methods (ultrasounds) and by phytochemical screening key secondary metabolites such as flavonoids and polyphenols, with antioxidant potential were identified in all the plants extracts. Antioxidant activity was quantified using the DPPH assay, and electrochemical behavior was assessed by cyclic voltammetry to detect redox-active compounds. The DPPH assay showed very good IC_{50} values for extracts of *Perilla spp.* which demonstrated the presence in the extracts of antioxidant compounds from the polyphenols class. Cyclic voltammetry revealed characteristic electron transfer peaks, especially in the methanolic extract (500 $mV \cdot s^{-1}$) and completed traditional DPPH tests successfully. The extracts obtained using NADES show higher anodic current values compared to the solvent over almost the entire potential range, which suggests the presence of electroactive species in the samples compared to the solvent. The combined approach of the two methods highlights the potential application of these natural compounds in food and pharmaceutical formulations.

Keywords: *Perilla spp.,* DPPH, ABTS, FRAP, cyclic voltammetry, antioxidant

References:

1. Ahmed, H.M.; Tavaszi-Sarosi, S. Identification and quantification of essential oil content and composition, total polyphenols and antioxidant capacity of Perilla frutescens (L.) Britt. Food Chem. 2019, 275, 730–738
2. A. J. Bard, L. R. Faulkner, and H. S. White, Electrochemical Methods: Fundamentals and Applications (3rd ed.), John Wiley & Sons (2022)

OP8

SOLVENT-DEPENDENT ELECTROCHEMICAL BEHAVIOR OF COPPER(I) COMPLEX-MODIFIED SCREEN-PRINTED SENSORS

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ABSTRACT

The modification of screen-printed electrodes with metal complexes has attracted increasing interest due to their tunable electrochemical properties and potential applications in sensing [1], [2]. The aim of this study was to modify and evaluate the electrochemical performance of two screen-printed sensors used as platforms for the immobilization of new copper(I) complexes, $[Cu(SCN)(PPh_3)(bq)]$ and $[Cu(SCN)(PPh_2py)(bq)]$ where PPh_3 (triphenylphosphine), PPh_2py (diphenylpyridylphosphine), and bq (bis(quinoline)) act as coordinating ligands. Electrode modification was performed using the drop-and-dry technique, and the influence of the dispersion solvent was investigated by comparing dimethylformamide and acetonitrile in order to obtain stable and reproducible films. The modified electrodes were characterized by electrochemical impedance spectroscopy (EIS) and cyclic voltammetry (CV) in a ferri/ferrocyanide solution, $[Fe(CN)_6]^{3-}/^{4-}$, used as a standard redox probe. EIS measurements indicated differences in interfacial properties depending on both the complex and the solvent. CV revealed well-defined redox processes, and analysis of key parameters (ΔEp, peak current ratio, and scan rate dependence) enabled comparison of electron transfer efficiency. The sensor modified with $[Cu(SCN)(PPh_3)(bq)]$ showed improved performance in acetonitrile, while $[Cu(SCN)(PPh_2py)(bq)]$ exhibited better stability and reproducibility when dispersed in dimethylformamide. These results highlight the important role of both the dispersion solvent and the metal complex structure in tuning the electrochemical response of screen-printed sensors.

Keywords: ligand; complex; solvent; reproducibility; sensitivity

References:

1. A. V. Bounegru, C. Iticescu, S. Butan, A. Ceoromila, și A. Tăbăcaru, „A novel electrochemical sensor modified with the $[Cu(SCN)(PPh_3)(dpa)]$ complex for the simultaneous detection of resorcinol and hydroquinone”, Sensing and Bio-Sensing Research, vol. 51, p. 100957, feb. 2026, doi: 10.1016/j.sbsr.2026.100957.
2. P. Ming et al., „An Electrochemical Sensor Based on Cu-MOF-199@MWCNTs Laden with CuNPs for the Sensitive Detection of Creatinine”, Langmuir, vol. 39, nr. 38, pp. 13656-13667, sep. 2023, doi: 10.1021/acs.langmuir.3c01823.

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OP9

VALORIZATION OF *NEOCARYA MACROPHYLLA* FRUITS BY MICROENCAPSULATION: PHYSICOCHEMICAL AND NUTRITIONAL CHARACTERIZATIONS

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ABSTRACT

Wild fruits play a crucial role in the management of malnutrition. This study aimed to enhance the value of *Neocarya macrophylla* fruits through microencapsulation using the freeze-drying technique. Starch was chosen as the wall material for preparing the microcapsules. Physicochemical and phytochemical characterization was performed. The encapsulation yield was 93.13%±0.013 with an efficiency of 39.52 ± 0.79%. Higher concentrations of biocompounds were registered with the microcapsules extracts, i.e. 83.40±2.28 mg GAE/100g for polyphenol and 40.05±0.55 mg CE/100g for flavonoids, respectively. The *in vitro* gastrointestinal test revealed that proteins were the most bioavailable compounds, with 79.82%±0.092 release during the intestinal phase. and The most stable compounds were flavonoids, which ranged from 0.39 to 0.36 mg EC/g DM. These results show that microencapsulation increases the bioavailability of nutrients contained in *N. macrophylla* fruits. In light of these results, it would be interesting to develop a food formulation based on these fruits.

Keywords: *Neocarya macrophylla*; microencapsulation; valorization

OP10

DETECTION OF VIRGIN OLIVE OIL ADULTERATION BY MEANS OF ELECTROCHEMICAL BIOSENSORS

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ABSTRACT

Virgin olive oil is obtained from olive fruits (Olea europea L.) by mechanical procedures and other physical means in conditions, especially thermal ones, that do not alter their properties [1]. Olive oil represents only 3.3% of the production of vegetable oils and fats, concentrating on olive production in the Mediterranean basin; approximately 75% of this production belongs to the countries of the European Union, mainly Spain and Italy [2]. The high market price and well-known health benefits attributed to virgin olive oil make this product a target for various types of fraud, such as adulteration by mixing it with other oils from different sources [3]. In this study different electrochemical biosensors based on nanomaterials (carbon nanotubes, carbon nanofibers and graphene) and enzymes (tyrosinase, laccase and peroxidase) were developed and used for the detection of phenolic biomarkers from virgin olive oils. The main biomarkers identified are tyrosol, hydroxytyrosol and oleuropein and the detection limits are in nanomolar range using differential pulse voltammetry. Furthermore, the voltammograms were used as input in multivariate data analysis and the classification models have shown adequate performances in detection of adulterated olive oils with rapeseed oils.

Keywords: virgin olive oil; nanomaterial; enzyme; biosensor

References:

1. Karagözlü, M., Adun, P., Ozsoz, M., Aşır, S., Detection of adulteration in cold-pressed olive oil by voltammetric analysis of alpha-tocopherol on single-use pencil graphite electrode. Int J Food Sci Tech 2024, 59, 1781–1788.
2. Contiñas, A., Martínez, S., Carballo, J., Franco, I., Detection of contaminations and/or adulterations of the extra virgin olive oil with seeds oils (sunflower and soybean) and olive pomace oil. Grasas aceites 2008, 59, 97–103.
3. Apetrei, I.M., Apetrei, C. Detection of virgin olive oil adulteration using a voltammetric e-tongue. Comput Electron Agric 2014, 108, 148–154.

OP11

DIOL-ASSISTED SYNTHESIS OF CuO NANOPARTICLES FOR IMPROVED ELECTROCHEMICAL SENSING OF H_2O_2

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ABSTRACT

A new non-enzymatic electrochemical sensor for H_2O_2 determination was developed by immobilization of copper (II) oxide nanoparticles (CuONPs) into matrix of poly(3,4-ethylenedioxythiophene) conducting polymer (PEDOT). CuONPs were synthesized through an additive-free polyol method and characterized by XRD, FTIR and UV-Vis methods. Drop casting of ethanolic CuONPs dispersion onto PEDOT matrix electrodeposited onto GCE by sinusoidal voltage method resulted in an organic-inorganic hybrid material with electrocatalytic properties toward H_2O_2 reduction. The sinusoidal voltage procedure supposed the application of a sinusoidal excitation voltage with a fixed frequency of 50 mHz and an amplitude of 0.25 V (rms) over a constant potential of +0.60 V. The deposition time was 20 min. The electrodeposition of the PEDOT coating using the sinusoidal voltage procedure was carried out from an aqueous solution containing 10 mM PEDOT monomer and 0.1 M KNO_3. The electrocatalytic performance of the PEDOT-CuONPs-based material was enhanced compared to the CuONPs-based material, showing improved electron transfer efficiency as well as superior overall analytical performance. The response of the electrode modified with PEDOT-CuONPs was linear over a concentration range of 0.04 to 10 mM for H_2O_2 with a low detection limit of 8.5 µM. The performance of the electrochemical sensor based on PEDOT-CuONPs was comparable to that of previously reported electrochemical sensors. The recovery values obtained from diluted milk samples ranged from 100% to 108%, indicating good accuracy and strong potential for real sample analysis.

Keywords: copper(II) oxide; hydrogen peroxide amperometric sensing; polyol method; sinusoidal voltage method; PEDOT

References:

1. Lete, C.; Spinciu, A.-M.; Alexandru, M.-G.; Calderon Moreno, J.; Leau, S.-A.; Marin, M.; Visinescu, D. Copper(II) Oxide Nanoparticles Embedded within a PEDOT Matrix for Hydrogen Peroxide Electrochemical Sensing. Sensors 2022, 22, 8252. https://doi.org/10.3390/s22218252

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2.POSTERS

SECTION VII: Workshop NOMARES NOUVEAUX MATERIAUX POUR LA RECONNAISSANCE ELECTROCHIMIQUE D'ESPECES INORGANIQUES ET BIOLOGIQUES (NOMARES 9th edition)/ New materials for the electrochemical recognition of minerals and biological species

PP1 Electrochemical Synthesis of Gold Nanowires for Interleukin 6 Detection

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ABSTRACT

The use of 1D metallic nanoarchitectures (i.e. nanowires, nanotubes, nanorods) are of great interest in the building of electrochemical sensors and biosensors thanks to their efficient electron transfer along 1D direction and good mechanical strength. They allow the fabrication of high-density nanoscale devices, too [1]. Gold nanowires (AuNWs) are of particular interest in this field and have been widely used as immobilization matrix in biosensors fabrication for enhancing their performance.

Herein, Au NWs using template-assisted method are developed, involving aqueous electrolytes. Cyclic voltammetry, chronoamperometry and chronopotentiometry have been applied as electrochemical techniques in order to get more information on the Au NWs deposition process. The electrochemically synthesized nanowires have been characterized using SEM and XRD investigations. Au NWs having about 90-110 nm in diameter and around 5-6 μm in length were formed as illustrated in Fig. 1.

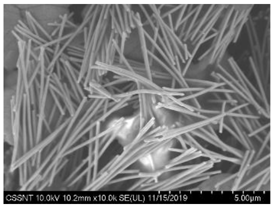

Fig. 1 – SEM micrograph of Au NWs electrochemically prepared at a cathodic potential E = -1.2 V *vs.* Ag/AgCl for 1000 s at 25°C

Interleukin 6 (IL-6) is a multifunctional cytokine influencing cancer cell activity, which is overexpressed in almost all tumor types. Its detection as a circulating tumor cells (CTCs) indicator is of major importance for the diagnosis and monitoring of the medical condition [2,3]. Therefore, preliminary results regarding the development of an impedimetric aptasensor for the detection of IL-6 by immobilizing it by multipulse-assisted amperometry (MPA) at the level of AuNWs that were immobilized on the graphite surface of printed planar electrodes (SPCE) are also presented.

Key words: Gold nanowires; electrochemical synthesis; electrochemical detection.

References:

[1] García, M., Batalla, P., Escarpa, A., Metallic and polymeric nanowires for electrochemical sensing and biosensing, Trends Anal. Chem. 2014, 57, 6–22.

[2] Tertis, M., Leva, P.I., Bogdan, D., Suciu, M., Graur, F., Cristea, C., Impedimetric aptasensor for the label-free and selective detection of Interleukin-6 for colorectal cancer screening, Biosens. Bioelectron. 2019, 137, 123–132.

[3] Tertiş, M., Ciui, B., Suciu, M., Săndulescu, R., Cristea, C., Label-free electrochemical aptasensor based on gold and polypyrrole nanoparticles for interleukin 6 detection, Electrochim. Acta. 2017, 258, 1208–1218.

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PP2 Effect of Co_3O_4 Doping on the Structure and Electrochemical Behavior of the 4Pb–PbO_2 System for Lead-Acid Battery Applications

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ABSTRACT

Lead-acid batteries remain attractive due to their low cost, robustness, and recyclability. Their performance is strongly influenced by the structure and electrochemical behavior of the active material. In this study, an experimental design was developed to investigate the effect of the Co_3O_4 addition on the $xCo_3O_4\cdot(100-x)[4Pb\cdot PbO_2]$ system with x = 0, 5, 10, 20, and 30 mol% Co_3O_4 prepared by melt-quenching method. Two parameters were controlled: the Co_3O_4 content and synthesis temperature. Three types of $4Pb\cdot PbO_2$ composition were prepared at 850, 900, and 950 °C, respectively to evaluate the effect of synthesis temperature on the host matrix. The selected temperature for the preparation of doped vitreous system was 900 °C due to the best macroscopic homogeneity of the sample. For the compositions containing up to 20 mole% Co_3O_4, the metallic Pb segregation was still visible, indicating that structural organization remained limited at these doping levels. In contrast, the sample containing 30 mole% Co_3O_4 exhibites a more compact and homogeneous morphology suggesting that higher Co_3O_4 contents promote better stabilization of the material.

The prepared materials were characterized by X-ray diffraction (XRD) and electron spin resonance (ESR). This study investigates also the electrochemical behavior of doped electrode system using cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS).

The XRD analysis evidences a vitroceramic structure containing PbO_2 and PbO at higher dopant levels and a small diffraction peak attributed to the formation of Co3O4 nanoparticles.. The ESR data show two resonance signals situated at about g ~ 2.08 and 4.3 due to the Co+2 ions. The first signal corresponds to the the Co+2 ions situated in the octahedral geometries while the second line provide the presence of Co+2 ions situated in the isolated tetrahedral positions. The presence of two signals represent an strong indicator for the formation of spinel Co3O4 crystalline phase with defects and the contributions of surface and inversion.

The cyclic volatmograms exhibit pronounced irreversibility characterized by the absence of well defined peak symmetry and significant peak separation, indicating sluggish electron transfer kinetics. EIS measurements reveal a progressive decrease in the diameter of the semicircle in Nyquist plots, corresponding to a reduction in charge transfer resistance. This behavior suggests that the doping enhances electrical conductivity and facilities charge transfer at the electrode – electrolyte interface. The sample with 30 mol% Co_3O_4 exhibites the lowest bulk resistance (Rb = 154 Ω) together with a favorable voltammetric response, indicating improved electrochemical performance.

The combined results demonstrate that while the electrochemical processes remain irreversible, doping effectively improves the electrochemical performance of the vitreous system by lowering resistance and promoting more efficient electron transport.

Key words: lead-acid batteries; Co_3O_4 doping; melt-quenching; electrochemical impedance spectroscopy; lead-based active materials.

PP3 Statistical Modeling and Measurement Validation for Electrochemical Data

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ABSTRACT

Electrochemical systems involve complex multiscale dynamics, including simultaneous mass transport and charge transfer. Traditional "best-fit" approaches often fail to account for system non-linearity and experimental artifacts. The objective of this work is to establish a framework that bridges theoretical electrochemistry with robust statistical validation , moving toward stochastic models that account for uncertainty in voltammetry and galvanostatic data.

The research utilizes several original families of molecular descriptors—such as FPIF, MDF, SMPI, SAPF, and ChFP—to encode chemical information and predict molecular characteristics through structure-property modeling. Validation is conducted via a suite of "home-made" statistical programs focusing on Normality and Outlier Detection (by applying tests based on the Cumulative Distribution Function (CDF) to identify data inconsistencies), Regression and Correlation Analysis (by utilizing linear and multi-variate regression alongside Pearson, Spearman, and Kendall correlation coefficients), and Monte Carlo Simulations (by employing advanced statistics including Anderson-Darling (AD), Cramér-Von Mises (CM), Kolmogorov-Smirnov (KS), Kuiper (KV), and Watson (WU) to calculate associated probabilities for continuous distributions).

The computational demand is extensive, as descriptor families like MDFV can generate over 2.3 million descriptors , leading to approximately 5·1013 evaluated sets for triple-descriptor linear regressions. To address this complexity, parallelization strategies are implemented using PHP and FreePascal. These tools distribute the calculation load across all available processors (CPUs), enabling the efficient processing of large datasets and ensuring rigorous statistical integrity for electrochemical models.

Key words: electrochemical complexity; molecular descriptors; structure-activity relationship; statistical validation; parallelization.

References:

[1]Jäntschi, L., 2004. MDF - A New QSAR/QSPR Molecular Descriptors Family. Leonardo J. Sci. 3(4): 68-85.
[2]Bolboacă, S. D., Jäntschi, L., 2006. Pearson versus Spearman, Kendall's Tau correlation analysis on structure-activity relationships of biologic active compounds. Leonardo J. Sci. 5(9): 179-200.
[3]Bolboacă, S. D., Jäntschi, L., 2008. Modelling the property of compounds from structure: statistical methods for models validation. Environ. Chem. Lett. 6(3): 175 - 181.

[4]Jäntschi, L., Bolboacă, S. D., 2018. Computation of probability associated with Anderson-Darling statistic. Mathematics 6(6): 88.

PP4 Applications of Chromatographic Methods in the Analysis of Ascorbic Acid in Pharmaceutical Products

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ABSTRACT

Ensuring the quality and stability of vitamins in pharmaceutical products is a major challenge for the industry, given the high sensitivity of these compounds to environmental factors. The present study focuses on the analysis of ascorbic acid (Vitamin C), an essential micronutrient with a critical role in human metabolic processes and immune system function.

The primary objective of this research was the development and validation of a precise analytical method for the identification and quantification of ascorbic acid in various pharmaceutical forms (infusion solutions, capsules, and tablets), including the monitoring of its integrity in products at or beyond their expiration date.

The study employed high-performance liquid chromatography (HPLC) in reversed-phase mode, using a system equipped with a UV-Vis detector ($\lambda = 240$ nm) and an Eclipse XDB C18 column. The optimized mobile phase consisted of a mixture of water, acetonitrile, and formic acid in a ratio of 94:5:1 (v/v/v). For result validation, a comparison was performed with the iodometric method based on oxidation with potassium iodate in the presence of starch.

The HPLC calibration curve exhibited excellent linearity within the concentration range of 5–100 mg/L, with a correlation coefficient of $r = 0.9989$. Analysis of pharmaceutical samples revealed variations between the measured and declared concentrations, particularly in expired products. The HPLC method proved superior to the classical chemical method by eliminating interferences caused by other reducing agents present in excipients.

The results confirm that HPLC is the optimal method for quality control of ascorbic acid, providing the sensitivity required to detect its degradation under the influence of temperature and light. The study highlights the importance of proper storage conditions in maintaining the bioactivity of vitamin C-based pharmaceutical products.

Key words: chromatographic methods, ascorbic acid, pharmaceutical products

PP5 Acute Cardiovascular and Respiratory Responses to High-Intensity Interval Training in Young Adult Women

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ABSTRACT

This study investigates the acute physiological responses to high-intensity interval training (HIIT) in a group of 40 female participants, with a mean age of 39.4 years, all of whom have been practicing sports for over 3 years and are members of a fitness center. The aim was to evaluate cardiovascular dynamics and respiratory function in response to exercise. Heart rate (HR) was recorded at multiple time points: pre-exercise and during effort at different stages of the training protocol. The mean resting HR was 77.9 ± 7 bpm, increasing to 136 ± 16 bpm during moderate effort and reaching 157 ± 14 bpm at higher intensity levels, indicating a significant cardiovascular response to HIIT. Pulmonary function was assessed using Forced Vital Capacity (FVC), which increased from 3.8 ± 0.2 L at baseline to 4.1 ± 0.3 L post-exercise, suggesting enhanced ventilatory involvement following physical effort. Additionally, heart rate variability (HRV) was monitored using a fitness device in order to explore autonomic nervous system responses to exercise; further analysis of this parameter is ongoing. The findings highlight the capacity of HIIT to induce substantial cardiovascular activation and acute improvements in respiratory parameters. These results support the effectiveness of HIIT protocols in enhancing cardiorespiratory function in trained adult women.

Key words: HIIT, heart rate, FVC, HRV, cardiovascular response, respiratory function

PP6 Azulene-thiadiazole 2D polymeric films as innovative electroactive materials for heavy metals sensing

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ABSTRACT

Azulene and 1,3,4-thiadiazole (TDA) are two structurally distinct building blocks whose combination offers a compelling platform for the development of advanced electroactive materials. Azulene's polarized non-benzenoid aromatic structure confers low ionization energy and high electron mobility, while TDA-containing derivatives contribute strong electron affinity, aromaticity, and chemical stability. Derivatives that contain TDA have a wide range of applications in medicine, organic electronics and electrochemistry [1-3].

In this work, three azulene monomers functionalized with TDA groups differing in their substituents were synthesized and used to fabricate chemically modified electrodes (CMEs) via direct electropolymerization onto glassy carbon substrates. Controlled-potential electrolysis was employed to deposit uniform two-dimensional (2D) polymeric films, and successful surface immobilization was confirmed using ferrocene redox probe assay. The electrochemical behavior of the monomers and the resulting CMEs was characterized by cyclic voltammetry, differential pulse voltammetry, and rotating disk electrode voltammetry, while surface morphology was assessed by scanning electron microscopy (SEM) and atomic force microscopy (AFM). SEM and AFM analyses revealed distinct surface topographies dependent on the nature and position of substituents, with electropolymerization conditions influencing film uniformity and thickness. The complexing capability of the CMEs toward heavy metal ions — Cd(II), Pb(II), Cu(II), and Hg(II) — was evaluated in aqueous solution using anodic stripping voltammetry. The results demonstrate that the azulene- thiadiazole CMEs exhibit sensitive and selective electroanalytical responses, with particularly strong performance for Pb(II) detection. These findings establish azulene-thiadiazole-based CMEs as promising, sensitive platforms for the development of electrochemical sensors for heavy metal ion sensing in environmental water matrices.

Key words: azulene-tetrazole; chemically modified electrodes; heavy metal sensing

References:

[1]Hu Y., Li C.Y., Wang X.M., et al. 1,3,4-Thiadiazole: Synthesis, Reactions, and Applications in Medicinal, Agricultural, and Materials Chemistry. Chem. Rev. 2014, 114(10), 5572-610.

[2]Chen H., Liu Z., Zhao Z., et al. Synthesis, Structural Characterization, and Field-Effect Transistor Properties of n-Channel Semiconducting Polymers Containing Five-Membered Heterocyclic Acceptors:

Superiority of Thiadiazole Compared with Oxadiazole. ACS Appl Mater Interfaces. 2016, 8(48), 33051-33059.
[3]Anăstăsoaie V., Omocea C., Enache L.-B., et al. Surface Characterization of New Azulene-Based CMEs for Sensing. Symmetry 2021, 13(12), 2292.

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PP7 Optical experiments and dft calculations for azulene-phenyloxazolones

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ABSTRACT

Oxazolones, also known as azlactones or oxazol-5(4H)-ones, are five-membered rings containing nitrogen and oxygen heteroatoms, demonstrated to be versatile scaffolds for various purposes in organic synthesis, due to the presence of pro-nucleophilic and electrophilic reactive sites in their structure [1], which consist basically of "masked" amino acids. Thus, oxazolones are important synthons for the synthesis of biologically active or peptidomimetic compounds. They became key monomer unit of various polymers and nanomaterials of biomedical uses [1-4] or an attractive heterocycle core of complex molecules with numerous biological or pharmaceutical applications, involved in several organic transformations [5] (ring-opening reactions, cycloadditions to form new carbon–carbon and/or carbon–heteroatom bond and to prepare various selective functionalized molecules, or conjugate additions, alkylation, allylation, arylation, acylation, etc.). Several substituted oxazolones based on 4-((azulen-1-yl)methylene)-2-phenyloxazol-5(4H)-one (O) were synthesized and characterized by elemental analysis, FT-IR, FT-Raman, 1H and 13C NMR spectroscopies [6]. Their concentration-dependent spectral behavior was investigated in acetonitrile by UV–Vis spectroscopy. Electrochemical experiments were also carried out by cyclic voltammetry, differential pulse voltammetry and rotating disk electrode voltammetry (CV, DPV, RDE) in presence of tetrabutylammonium perchlorate as supporting electrolyte on glassy carbon electrode [7]. The UV–Vis spectra showed a clear concentration-dependent increase in solutions absorbance, allowing the construction of linear calibration curves. This study extended the characterization of these azulene-phenyloxazolones. The DFT calculation was correlated with the experimental results obtained by UV–Vis and with the performances of CMEs obtained using ligands with different substitulents related to O. This study is relevant for further design and development of advanced materials based on az-ulenyl-phenyloxazolone for the analysis of HMs in water.

Key words: Azulene-phenyloxazolones, Optical experiments, DFT calculations, Chemically modified electrodes.

References:

[1] P.P. De Castro, A.G. Carpanez, G.W. Amarante, Chem. Eur. J. 2016, 22, 10294–10318. https://doi.org/10.1002/chem.201600071Digital Object Identifier (DOI)

[2] Y.M. Zayas-Gonzalez, B.J. Ortiz, D.M. Lynn, Biomacromolecules 2017, 18, 1499–1508. DOI: 10.1021/acs.biomac.7b00043
[3] X. Wang, J.L. Davis, B.M. Aden, B.S. Lokitz, S.M. Kilbey, Macromolecules 2018, 51, 3691–3701. https://pubs.acs.org/doi/10.1021/acs.macromol.8b00405
[4] C. Chauveau, E. Vanbiervliet, S. Fouquay, G. Michaud, F. Simon, J.-F. Carpentier, S.M. Guillaume, Macromolecules 2018, 51, 8084–8099. https://pubs.acs.org/doi/10.1021/acs.macromol.8b01628
[5] I.F.S. Marra, P.P. de Castro, G.W Amarante, Eur. J. Org. Chem. 2019, 5830–5855. https://doi.org/10.1002/ejoc.201901076
[6] M. Cristea, L. Bîrzan, F. Dumitrascu, C. Enache, V. Tecuceanu, A. Hanganu, C. Draghici, C. Deleanu, A. Nicolescu, M. Maganu, et al. Symmetry 2021, 13, 1209. https://doi.org/10.3390/sym13071209
[7] A.-G. Brotea, O.-T. Matica, C. Musina (Borsaru), M. Cristea, A. Stefaniu, A.-M. Pandele, E.-M. Ungureanu, Symmetry 2023, 15, 540. https://doi.org/10.3390/sym1502054

PP12 Aminoglycoside Antibiotic Detection Using a Diazonium-Electrografted Aptasensing Platform

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ABSTRACT

Antibiotics are extensively used in clinical and veterinary practice, making their reliable detection essential for food safety, environmental, and biomedical monitoring. Electrochemical aptasensors represent a promising approach for this purpose, as they combine the molecular recognition capability of aptamers with the sensitivity and simplicity of electrochemical transduction. In this study, we report the electrochemical detection of three aminoglycoside antibiotics, based on an optimized aryldiazonium-derived aptasensing platform developed in our previous studies1,2. The sensing platform was fabricated at glassy carbon electrodes through the electrochemical reduction of 4-[(triisopropylsilyl)ethynyl]benzene diazonium tetrafluoroborate, following a protected aryldiazonium salt electrografting strategy for suppressing the formation of disordered polyaryl multilayers. The resulting phenyl-ethynyl functionalized surface was further used for the covalent immobilization of an ssDNA aptamer sequence with tobramycin specificity3. The aptamer was designed with two terminal modifications: a 5′-azidobutyrate group and a 3′-methylene blue (MB) label. Immobilization at electrode was achieved through an azide-alkyne click reaction between the surface tethered ethynyl groups and the 5′-azidobutyrate modification of the aptamer. The 3′-MB label acted as a redox reporter, enabling SWV monitoring of analyte concentration through target-induced aptamer conformational rearrangement and altered electron transfer at the electrode interface. The electrochemical response was evaluated at different SWV interrogation frequencies, and the aptamer-target equilibration time was optimized by monitoring the MB signal. Tobramycin, kanamycin, and streptomycin were successfully detected at this platform, with sensitivities depending on the target antibiotic. The influence of SWV frequency on the analytical response was also target-dependent, indicating that the interrogation conditions must be optimized individually for each aminoglycoside. Under optimized conditions, calibration curves showed linear responses over the concentration range of $5 \cdot 10^{-7}$ to $5 \cdot 10^{-4}$ M.

Key words: aptasensor; aryldiazonium salts; electrochemical functionalization; antibiotic

References:

[1]Onaş, A.M.; Pandele, A.M.; Hanganu, A.; Florea, C.V.; Marton, G.; Iovu, H.; Raicopol, M.D.; Pilan, L. Controlled surface functionalization using aryldiazonium salts with bulky protecting groups for the development of DNA-based sensing platforms, Surfaces & Interfaces, 2024, 46, 103855.

[2]Onaş, A.M.; Pandele, A.M.; Hanganu, A.; Florea, C.V.; Iovu, H.; Raicopol, M.; Pilan, L., Facile preparation of bifunctional monolayers through diazonium grafting and "click" postfunctionalization: A first step towards efficient aptasensing interfaces, Bioelectrochemistry, 2025, 163, 108904.

[3]Rowe, A.A.; Miller, E.A.; Plaxco, K.W. Reagentless measurement of aminoglycoside antibiotics in blood serum via an electrochemical, ribonucleic acid aptamer-based biosensor, Anal. Chem. 2010, 82, 7090-7095.

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PP13 Hybrid Materials-Based Electrochemical Sensing Platforms for Biomolecules

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ABSTRACT

Owing to its strong adhesive properties, polydopamine (PDA) is highly effective as a universal surface modifier. PDA contains various functional groups, including catechol, amine, and quinone moieties, which enable it to participate in further reactions such as metal ion chelation, covalent coupling, and secondary functionalization with biomolecules or nanoparticles. PDA improves electron transfer, provides abundant active sites, and can stabilize immobilized catalytic species such as metal nanoparticles or enzymes [1].

In this work, the in-situ preparation, characterization, and analytical applications of hybrid materials containing polydopamine are presented. The hybrid material has been prepared by a range of methods, including classical cyclic voltammetry as well as new procedures using alternate currents. The electrodic substrate was made of glassy carbon. The preparation methods could also be applied to other substrates such as platinum, gold and/or carbon-based screen-printed electrodes. The electrochemical synthesis parameters were optimized through a feedback approach employing a redox-active soluble probe in combination with cyclic voltammetry. The developed electrochemical sensing platforms were applied successfully in the detection of some bioactive compounds in synthetic samples [2]. High accuracy, negligible matrix effects, and competitive analytical performance were obtained in real sample analysis.

Key words: hybrid material; polydopamine; alternate currents; sensing platform.

References:

[1] Ryu J.H., Messersmith P.B., Lee H. Polydopamine surface chemistry: A decade of discovery. ACS Appl. Mater. Interfaces 2018, 10(9), 7523–7540.

[2] Leau S.-A., Lete C., Matei C., Lupu S. Novel biomimetic polymer-based material prepared by alternate currents method for electrochemical sensing platform development. J. Electroanal. Chem. 2026, 1001, 119703.