Book of Abstracts

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Forward

NInTec association brings together researchers and staff involved in research activities across the broad and diverse scientific ecosystem under the auspices of Instituto Superior Técnico.

Following the success of its first edition, NInTec is very pleased to announce the second edition of NInTec Science Days, an interdisciplinary event aiming at sharing knowledge, experience, and some of the latest research developments within the Técnico community. The event is an opportunity to promote cross-fertilization between different scientific areas as well as to establish dialogues between different stakeholders. Thus, the participation of PhD students and Técnico alumni following research careers in industry, SMEs, and business firms is also highly encouraged.

In this edition, we have awarded the Best Student Contribution, with a monetary incentive to the presenter*. The NInTec Science Days 2024 Best Student Contribution was awarded to Hemaxi Narotamo and her presentation on "Artificial Vision: Analysing Mouse Eye Blood Vessels with AI"*

NInTec Science Days 2024 also addressed science policy issues in parallel with the main scientific program. This second edition focused on the **"Evaluation Methods for Researchers and Research Assessment"**. The event promoted a round table in this topic, including a panel of invited speakers and the participation of the audience.

NInTec acknowledges the support from Pastéis de Belém, Labor Spirit, Grupo ILC, Impersol, Hugo O'Neill (Graphic Designer), and Instituto Superior Técnico. Check our sponsors in this link.

More information about the event can be found here.

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SCIENCE DAYS 24
OCT 28-29 Lisbon

Contents

Scientific Programme

Monday, October 28

10:00 - 10:20 Opening Session

10:20 - 11:20 First Scientific Session - Chair: Pedro Paulo

10:20 - Théo Abounnasr-Martins - A Tale of Two-Streams, Light and the Invisible Axion

10:40 - Carlo Alfisi - Plasmonic instability for ultra-low energetic weakly interactive particle detection

11:00 - Ricardo Jorge Clemente Martins - Simulation and experimental production of (FeTiTaA)(1-x)Wx (A = Cu, V, Cr) high entropy alloys

11:20 - 11:50 Coffee Break

11:50 - 12:50 Second Scientific Session - Chair: Ana Margarida Ricardo

11:50 - Hemaxi Narotamo - Artificial Vision: Analysing Mouse Eye Blood Vessels with AI

12:10 - Madalena Antunes - A 3D-printed clamping interface for tensile testing of biological specimens

12:30 - João Rodrigues - Organic Electroactive Molecules for Next-Generation Batteries, an exploratory approach with the tetrathiafulvalene derivatives.

Lunch Break

14:30 - 15:30 Third Scientific Session - Chair: Nuno Cruz

14:30 - Joana Pereira - Strategies for the separation of thorium from uranium using functionalized ionic liquids

14:50 - Carolina Dantas - Application of Machine Learning Techniques to Reflectometry Signals in Nuclear Fusion Plasmas

15:10 - Gustavo Maia - Impact events of extraterrestrial bodies: The bridge between exogenous delivery and the origin of life

15:30 - 16:00 Coffee Break

16:00 - 17:30 Scientific Poster Session

#1 Francisco Cruz Artificial Neural Networks for RBS Spectra Analysis

#2 Pietro Civa Exploring Deep Eutectic Solvents in Palladium Environmental Analysis: A First Look

#3 Cláudia Ribeiro - Pre-targeting bioorthogonal strategy for tethering photoactive BODIPY onto the plasma membrane of HER2+ gastric tumours

#4 João Alcobia Valorization of Arbutus unedo Bagasse using Eutectic Solvents for Cosmetic Applications

#5 Maria Serralha Supercritical antisolvent microencapsulation of oil extract from microalgae Cryphtecodinium cohnii

#6 David Graça Photoinduced Plasmon-assisted Functionalization of Gold Nanorods for Improved Plasmon-based Sensors

#7 Silvia Buriac Fluxes of Mercury and Methylmercury in Thermokarst Lakes

#8 Margarida Gonçalves Impregnation of soft contact lenses using supercritical fluids

#9 Vicente Guerreiro Determining the rhizosphere influence of Halimione portulacoides on mercury concentration and bacterial diversity in the saltmarsh sediments of the Tagus Estuary (Lisbon)

#10 Sofia Marques Effect of plants on mercury dynamics in permafrost thaw systems

#11 Inês Rico Spatio-temporal assessment of variations in mercury levels in saltmarsh regions of the Tagus and Guadiana estuaries

#12 Daniel Agostinho Experimental Wind Turbine Simulator

#13 Luís Alves Ion Beam Analytical techniques combined for the characterization of cultural heritage material

#14 Raquel Cabaça Microencapsulation of a Far-Red absorbing Phthalocyanine: recent advances on microscale engineering of polyelectrolyte multilayers

Tuesday, October 29

10:00 - 11:00 Fourth Scientific Session - Chair: José Vicente

10:00 - Filipe da Silva - Modelling Reflectometry Diagnostics: Finite-Difference Time-Domain Simulation of Reflectometry in Fusion Plasmas

10:20 - Hugo Terças - Axions in plasmas and metamaterials

10:40 - Nuno Cruz - New Operation and Collaborative Tools for Advancing ITER Neutral Beam Test Facility Research

11:00 - 11:30 Coffee Break

11:30 - 12:30 Fifth Scientific Session - Chair: Beatriz Nobre

11:30 - Maria Jeremias - Improved voltammetric method for detecting Pd and Ni simultaneously using signal transformation

11:50 - José Santos / Pedro Paulo - DNA Origami Tetrahedra for Positioning of Plasmonic Gold Nanorods Antennas

12:10 - Rute Cesário - Distribution Patterns and High-Concentration Areas of Metal Pollution in Soils from Fildes Peninsula, King George Island, Antarctica

Lunch Break

15:00 - 17:00 Round Table - "Evaluation Methods for Researchers and Research Assessment".

17:00 - 17:30 Closing Session and Award Ceremony

October 28 - Oral Sessions

A Tale of Two-Streams, Light and the Invisible Axion

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In this talk, I will introduce the subject of plasma instabilities at the intersection of astrophysics, plasma and particle physics.

I will explore the prevalence of the 'two-stream' instability in space plasmas and its crucial role in shaping the space environment as we observe it, and beyond. This instability marks the beginning of a complex and turbulent dynamic process that can accelerate particles to energies equal to or greater than those produced by technological accelerators. The observable effects include electromagnetic radiation (light) and the arrival of energetic nuclei on Earth (cosmic rays). Plasma instabilities, therefore, are instrumental in illuminating the sky with phenomena ranging from the brightest cosmic explosions to the polar lights observed near Earth.

I will present the challenge that plasma instability poses to theoretical understanding, and the unexpected opportunity it offers to bring to light particles of Dark Matter – specifically, the invisible axion model - through complex interactions with plasma waves.

While sharing this scientific account, I will attempt to reflect on the benefit of international and cross-disciplinary collaboration on the development of my research at IST.

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Plasmonic instability for ultra-low energetic weakly interactive particle detection

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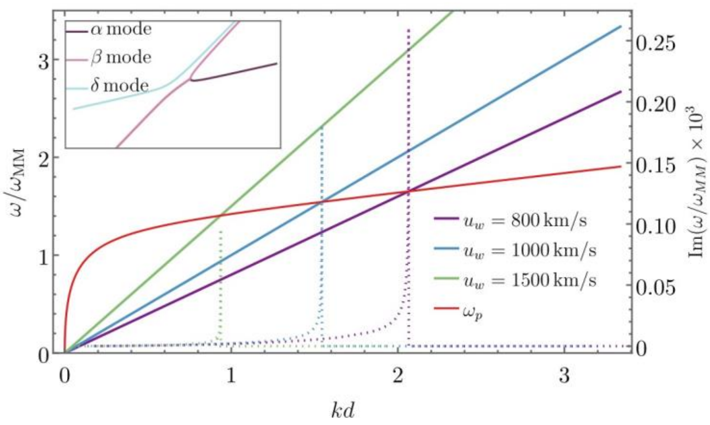
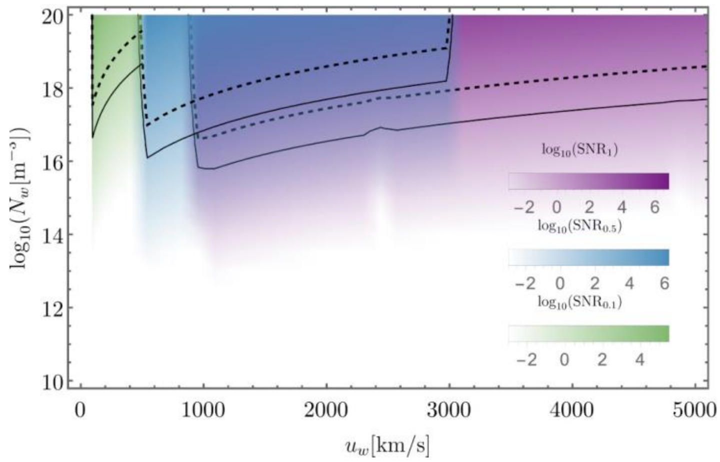
To test theories beyond the Standard Model, we need data for validation. A key area of interest is the neutrino sector and, more broadly, the class of Weakly Interacting Massive Particles (WIMPs). In a plasma environment, WIMPs interact with electrons via charged and neutral weak bosons (W and Z), leading to instabilities that trigger the growth of plasmonic waves. These electron oscillations carry information about WIMPs and can influence their propagation. In the case of neutrinos, the plasmons may even interfere with flavour oscillations (beyond MSW effect). Our preliminary work focused on plasmon growth in a graphene multilayer metamaterial subjected to a monochromatic WIMP flux, with characteristics compatible with the Dark Matter Halo.
The results indicate that the instability growth rate scales with $G_F^{2/3} N_p N_w / M_e E_w$, where G_F is the Fermi Constant, N_p (N_w) is the plasma (WIMP) density, M_e is the electron mass and E_w is the WIMP energy.





On the image to the left, we depict the plasma mode of a metamaterial (w_p) alongside the mode of WIMP at different velocities (u_w), the dotted lines represent the imaginary part of the resulting complex frequency i.e., the growth rate. The image to the right shows the Signal-to-Noise Ratio (SNR), defined as the plasmon energy over the thermal energy, as function of the WIMP speed and density for three detectors (w_p = [1, 0.5, 0.1] THz), The solid line highlights SNR=10, while the dashed line represents SNR=20.

The goal of this work is to share insights on the WIMP-plasma interactions with the community, aiming to address the significant challenges this topic will encounter:

1. The need of a fully self-consistent quantum theory to study the WIMP-Plasma interaction
2. Identifying the optimal plasma to maximize the resonance
3. Designing a detection scheme to fully characterize the generated plasmons
4. Investigating how plasma oscillations affect the MSW effect in the case of neutrino flux.
5. And more

Keywords: Plasmonic, WIMP, ultra-low energy, resonant instability, Beyond Standard Model

Simulation and experimental production of $(FeTiTaA)_{(1-x)}W_x$ (A = Cu, V, Cr) high entropy alloys

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High Entropy Alloys, with their complex compositions and exceptional properties, demand simulation techniques to understand their behavior. This work employs Molecular Dynamics and Monte Carlo simulations to provide a better understanding and comprehension on the $(FeTiTaA)_{(1-x)}W_x$ (A = Cu, V, Cr) high entropy alloys phase formation.

Monte Carlo and Molecular Dynamics simulation results show that for all systems achieved one single BCC type structure with random distribution of the elements. The Molecular Dynamics simulation results for the three alloy systems, shows the inexistence of chemical segregation corresponding to a small standard deviation, approximately constant with temperature, reflecting the random distribution of the elements in the structure. On the other hand, Monte Carlo simulation, displays lower potential energy for all systems, however for CuFeTiTaW system the simulation resulted in two different phase separations, for FeTiTaVW and $(CrFeTaTi)_{70}W_{30}$ alloys element segregation was attained at high temperatures.

The microstructural analysis of the consolidated CuFeTiTaW sample displays Fe-rich phase and a Cu-rich which is predicted for Monte Carlo simulation. Moreover, the microstructural analysis for both FeTiTaVW and $(CrFeTaTi)_{70}W_{30}$ systems evidenced presence of a Ti and W-rich phases in agreement with Monte Carlo simulation. In all systems can be observed two phases: one W-rich phase and a major phase with homogeneous element distribution which should correspond to a BCC type structure predicted by X-ray diffraction.

Therefore, it can be concluded, that Monte Carlo simulations results seems to be in agreement with the experimental results with the respect of the understanding the thermodynamic stability and the segregation behavior of (FeTiTaA)(1-x)Wx (A = Cu, V, Cr).

Keywords: Nuclear fusion reactor; High entropy alloys; Simulation

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Artificial Vision: Analysing Mouse Eye Blood Vessels with AI

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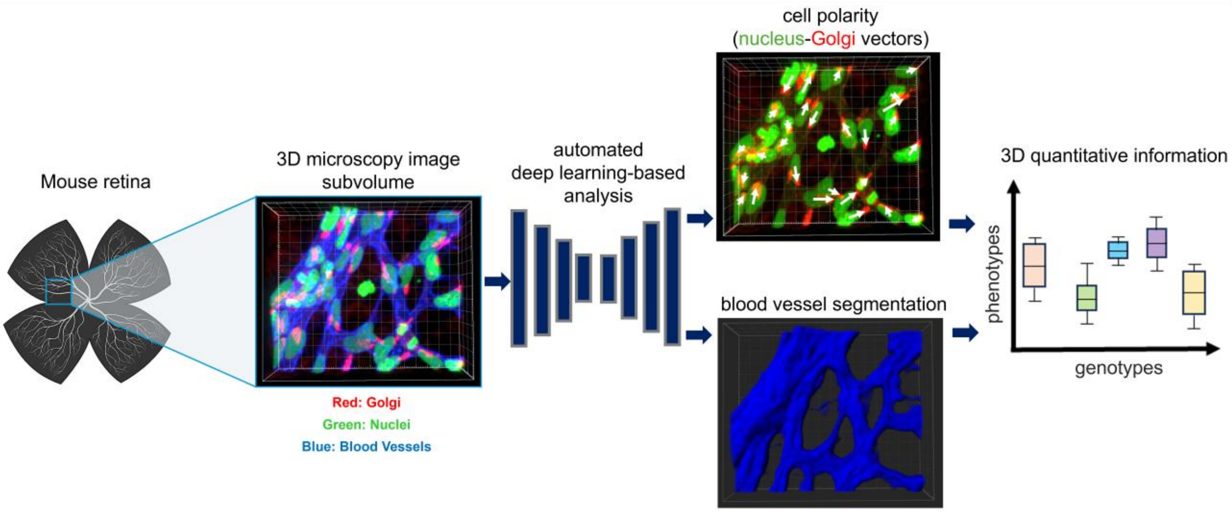
Blood vessels provide oxygen and nutrients to all tissues in the organism, and their dysfunction contributes to diseases, such as retinopathies and cancer. Formation of new blood vessels (angiogenesis) occurs in two steps: (i) Sprouting angiogenesis, which creates a primitive vascular network; and (ii) Vascular patterning, which remodels primitive networks into their hierarchical and functional branched pattern. However, the signalling pathways and molecular/cellular mechanisms associated to vascular patterning are poorly understood.

Previous works based on the analysis of microscopy images of mouse retinas have shown that endothelial cells (ECs), the cells lining the inner surface of vessels, polarize and migrate against the blood flow during vascular patterning. EC polarity is defined as a vector from the nucleus to the Golgi centroid. These conclusions have been drawn based on 2D studies of the mouse retinal vasculature thus they neglected the 3D structure of ECs and blood vessels. Moreover, the methods proposed in these works require manual nucleus-Golgi vectors annotation and semi-automatic blood vessels segmentation, which are laborious tasks performed by experts.

To circumvent limitations of previous works, we have developed automated deep learning-based approaches to compute 3D nucleus-Golgi vectors and segment 3D blood vessels in microscopy images of mouse retinas. We have validated the proposed methods on datasets containing images and respective ground-truth. The major contribution of the proposed approaches compared to previous works is that our methods perform large scale analysis in 3D in an automated manner. Furthermore, we present a freely available software that includes a user-friendly graphical interface for researchers with no programming experience, which will greatly facilitate the ability to study vascular networks in 3D in health and disease.

In the future, the proposed pipeline will be used to automatically extract several morphological features, associated to blood vessels and ECs, from mouse retinas at different stages of development and under different conditions. Hence, our work will try to answer open questions in vascular biology mainly associated with the process of vascular patterning using the proposed automated methods for 3D microscopy image analysis.

Figure/Scheme:



Keywords: deep learning, 3D microscopy images, mouse retinal vasculature, graphical user interface

A 3D-printed clamping interface for tensile testing of biological specimens

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Tensile testing of soft biological specimens is challenging. When compressed by the grips, the reduction in specimen thickness and interface adherence may lead to slippage and failure at the sharp grip edges. Several modifications have been proposed to address these issues [1,2]; however, they are not free of limitations [2]. The purpose of this study was to design a clamping interface to improve specimens' adherence to the grips and prevent tissue damage at the grip region. The clamping interface was designed considering the dimensions and structural constraints of the grips. Manufactured through additive manufacturing with PLA, it serves as an interface for the pneumatic grips. Four contact patterns were designed: retrograde teeth, serrated, atraumatic, and flower. Uniaxial tensile tests were performed using porcine skin specimens (n=5) for seven test conditions (Figure 1). For each trial, the maximum force (N) supported by the specimens (before slippage or failure) and failure location were determined. No difference was found between the reference and sandpaper test conditions. Compared to the reference condition, there was a significant improvement for the retrograde teeth and flower patterns ($p<0.01$). The clamping interface promoted failure in the testing region. The 3D-printed clamping interface significantly improved the adherence of the specimens to the grips, enabling the maximum capacity of the grips to be reached, and prevented damage at the grip region. The design of the clamping interface allowed to mitigate the issues commonly reported in the literature for tensile testing of soft tissues. Furthermore, the design can be easily customized to fit the available grips, and its production is fast, cost-effective, and easily accessible.

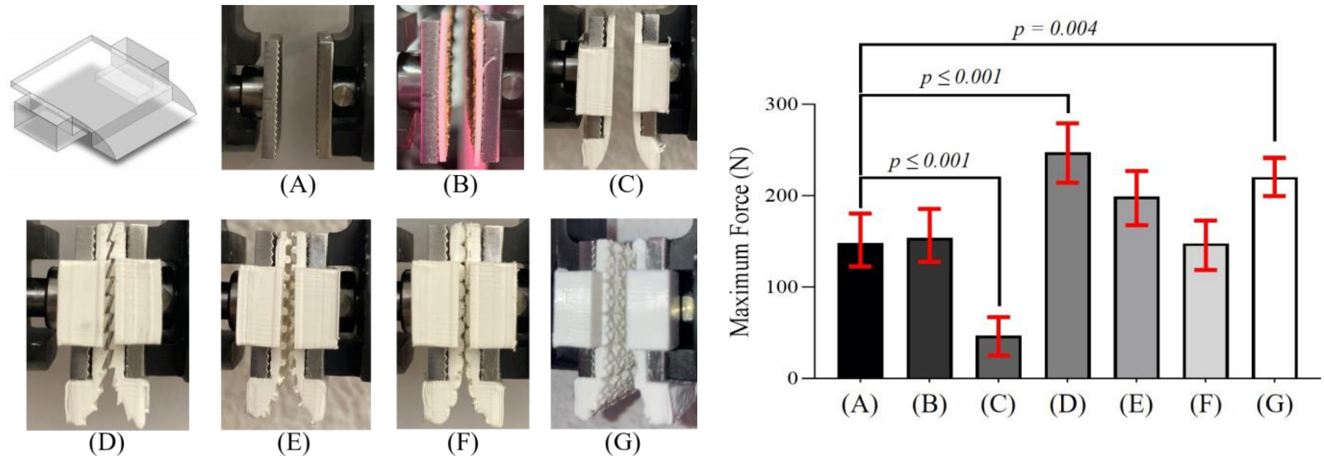

Figure 1: Clamping interface with test conditions (on the left): (A) reference; (B) sandpaper; clamping interface with (C) no contact pattern, and with the (D) retrograde teeth, (E) serrated, (F) atraumatic, and (G) flower patterns. The maximum force (N) supported by the porcine tensile specimens is shown on the right.

Keywords: Soft tissue, uniaxial tensile testing, specimen slippage, grips, additive manufacturing.

Acknowledgments: The authors acknowledge Fundação para a Ciência e a Tecnologia (FCT) for its financial support via the project LAETA Base Funding (DOI: 10.54499/UIDB/50022/2020), and a PhD scholarship 2021.06844.BD.

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1. C. Sang et al, J. Biomech Eng, 140, 2018.
2. M. Jiang et al, J Mech Behav Biomed Mater, 103:1751-6161, 2019.

Organic Electroactive Molecules for Next-Generation Batteries, an exploratory approach with the tetrathiafulvalene derivatives.

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Tetrathiafulvalene (TTF) is an electroactive organic compound being studied for various applications, including as a cathode material. This work focuses on the synthesis and characterization of the electrochemical behavior of TTF derivatives in aqueous electrolytes. The study of different organic compounds as electrodes could have benefits for battery manufacturing: increased environmental friendliness, higher safety, lower costs, and simpler processing at the end-of-life stage. However, organic electroactive materials suffer from low electronic conductivities, which lead to lower practical specific capacities, as well lack of structural stability.

This work seeks to study the potential of TTF derivatives as cathode materials through cyclic voltammetry (CV), testing all compounds in the same electrolyte (lithium nitrate), as well as testing in different concentrations of the same electrolyte to understand the redox reactions undergone at different potentials and in electrolytes with different counter-cations (potassium nitrate), to assess the potential of these materials in different battery chemistries.

While the compounds studied suffer from low electronic conductivities, as well as being electroactive at potentials at which water decomposes, and the redox processes observed are not yet fully understood, this work helps lay the groundwork for future studies of these compounds or other TTF derivatives, as one of the advantages of these compounds is the simple and intuitive synthesis process with high flexibility in terms of molecular structure, allowing for a high variety of TTF derivatives to be synthesized.

Keywords: Tetrathiafulvalene, Organic electroactive materials, Aqueous batteries

Strategies for the separation of thorium from uranium using functionalized ionic liquids

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Thorium is tagged to be a next-generation nuclear fuel since it is more abundant than uranium and produces less long-lived nuclear waste compared to uranium fuel [1]. Fertile ^{232}Th is converted to fissile ^{233}U in the nuclear reactor and, to accomplish a closed fuel cycle, reprocessing of spent nuclear fuel and separation of thorium and uranium are required. As a separation technology, liquid-liquid extraction with ionic liquids (ILs) is a promising strategy for advanced nuclear fuel cycles. Compared to conventional organic compounds, ILs are superior for their high tunability, thermal stability, wide liquidus range, and higher stability against radiation. The introduction of binding groups with high affinity for metals, in the cationic or anionic unit, is expected to enhance extraction efficiency and selectivity.

Previously, our group verified that three functionalized ILs (FILs) with a carboxylate or an oxamate moiety (see Fig. 1), dissolved in toluene, were able to extract lanthanides from aqueous solutions, with $[N_{8888}]$[DEHOX] displaying high selectivity along the lanthanide series [2]. In this work, we evaluated the ability of these FILs to extract selectively thorium and uranium from acidic aqueous solutions. $[N_{8888}]$[OL] exhibited higher extraction selectivity for UO_2^{2+} ions into toluene, with an extraction efficiency of 89% and distribution ratios ($D = [An]_{org}/[An]_{aq}$) of 0.54 and 8.16 for Th(IV) and U(VI), respectively, at pH = 3 and molar ratio 5:1 (IL:An). $[C_4mim]$[DEHOX] exhibited higher selectivity for Th(IV), with an average extraction efficiency of 97% and distributions ratios of 60.0 and 0.18 for Th(IV) and U(VI), respectively, at pH = 3 and molar ratio 3:1, while $[N_{8888}]$[DEHOX] extracted both actinide ions with similar efficiencies. These results are based on X-ray fluorescence (XRF) analyses of both organic and aqueous phases, which were corroborated by Inductively Coupled Plasma Mass Spectrometry (ICP-MS) analyses of calibration solutions.

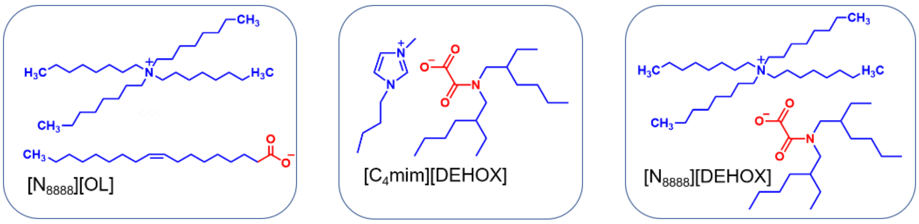

Figure 1. Chemical structures of the used FILs.

Keywords: thorium nuclear fuel, thorium(IV), uranyl(VI), liquid-liquid extraction, ionic liquids.

References:

[1] *Perspectives on the Use of Thorium in the Nuclear Fuel Cycle*, Nuclear Energy Agency, 2015.
[2] L. Maria, A. Cruz, J. M. Carretas, B. Monteiro, C. Galinha, S. S. Gomes, M. F. Araújo, I. Paiva, J. Marçalo, J. P. Leal, *Sep. Purif. Technol.*, 2020, 237, 116354.

Acknowledgments: This work was supported by FCT through projects UIDB/00100/2020 (CQE), LA/P/0056/2020 (IMS), and UIDB/04349/2020 (C^2TN).

APPLICATION OF MACHINE LEARNING TECHNIQUES TO REFLECTOMETRY SIGNALS IN NUCLEAR FUSION PLASMAS

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Hot plasmas are the medium where nuclear fusion reactions occur in stars and in experimental fusion devices using magnetic confinement. To monitor and control the plasma in nuclear fusion reactors, it is necessary to measure the electron density of the plasma. One of the diagnostic techniques used for this purpose is microwave reflectometry [1]. This technique is based on sending waves with specific frequencies to probe the plasma, propagating through regions of increasing density until reaching a critical layer of plasma density where the wave is reflected. The reflected wave undergoes a phase shift equivalent to the time delay of a radar echo. The temporal variation of this delay is related to a beat frequency of the interference signal obtained at the reflectometer's detector. However, plasma turbulence and other noise sources complicate the extraction of the beat frequency. In this work, with the goal of improving the measurements obtained with this type of reflectometry diagnostics, machine learning techniques are explored, and neural networks are developed and applied to reflectometry data [2]. The use of neural networks can enable more automated plasma diagnostic processes and real-time control of its position in future nuclear fusion reactors. For the training, testing, and validation of the machine learning models, experimental data from the ASDEX Upgrade magnetic confinement device were used [3]. The first results of applying these models for estimating beat frequencies are presented, which allow the reconstruction of the electron density profile of the probed plasma.

[1] T. Estrada, *et* al., Plasma and Fusion Research, **7** (2012) 2502055
[2] J. Santos, *et al.*, Fusion Eng. Des. **48-1** (2000) 119-126
[3] ASDEX Upgrade Special Issue, Fusion Science and Technology **44** (2003) Issue 3.

Keywords: Neural Network, Nuclear Fusion Plasma, Microwave Reflectometry, Electron Density, Beat Frequency

Impact events of extraterrestrial bodies: The bridge between exogenous delivery and the origin of life

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With the discovery of nucleobases, ribose, and other organic molecules among meteorite extracts, extraterrestrial delivery has been pointed out as one important prebiotic source for the synthesis of relevant organic molecules.[1] It´s assumed, due to their stability, that most of these molecules are brought directly from outer space. Currently, *The RNA World Hypothesis*, which states that life began with small RNA-like moieties, is the most accepted model for the origin and evolution of life on Earth.[2] Ribonucleosides, the building blocks of RNA, were yet not found among extraterrestrial samples, opposing its components (i.e. nucleobases and ribose).[1] In addition to that, the direct condensation of ribose and nucleobases, to give RNA building blocks, ribonucleosides, and ribonucleotides, is not a sustainable prebiotic reaction.[2]

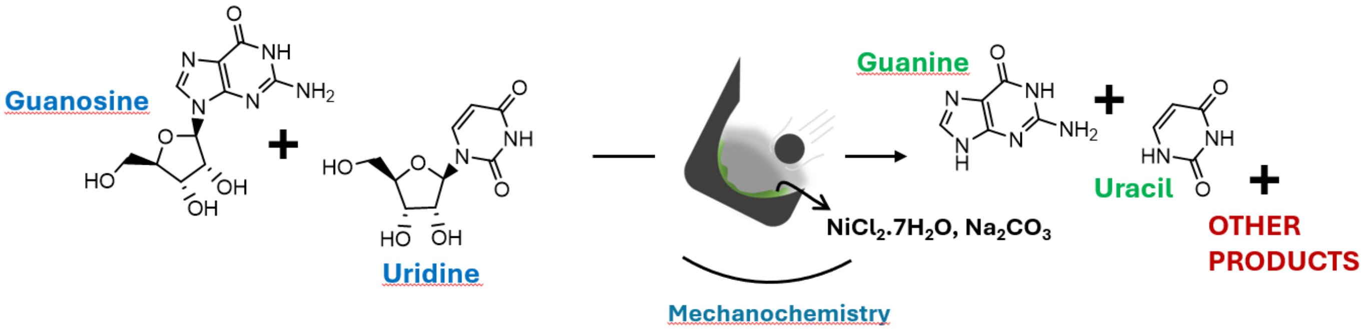

Figure 1 – Mechanochemical degradation model of ribonucleosides in their respective nucleobases in the presence of metal salts.

Herein, it is proposed a different point of view regarding exogenous delivery, stating that the degradation of complex organic molecules, through mechanochemical reactions, is a plausible explanation for the lack of nucleosides and peptides among meteorite extracts. DFT methodologies will be implemented to predict the degradation mechanisms and new detection methodologies are being optimized for meteorite and asteroid samples. Until now, the mechanochemical degradation of canonical ribonucleosides (adenosine, guanosine, cytidine, and uridine), induced by metals (high Lewis's acidity, such as Al^{3+}, Fe^{2+}/Fe^{3+}, and Ni^{2+}) and carbonate (i.e. CO_3^{2-}) ions was accomplished.[3] In addition to that, purine and pyrimidine HPLC-UV/MS separation has been partially optimized. This work can lead to new insights regarding the origin of life (i.e. prebiotic chemistry) that might be further explored in future space missions.

Keywords: Meteorites; Asteroids; Mechanochemistry; Exogenous Delivery

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October 28 - Poster Session

Artificial Neural Networks for RBS Spectra Analysis

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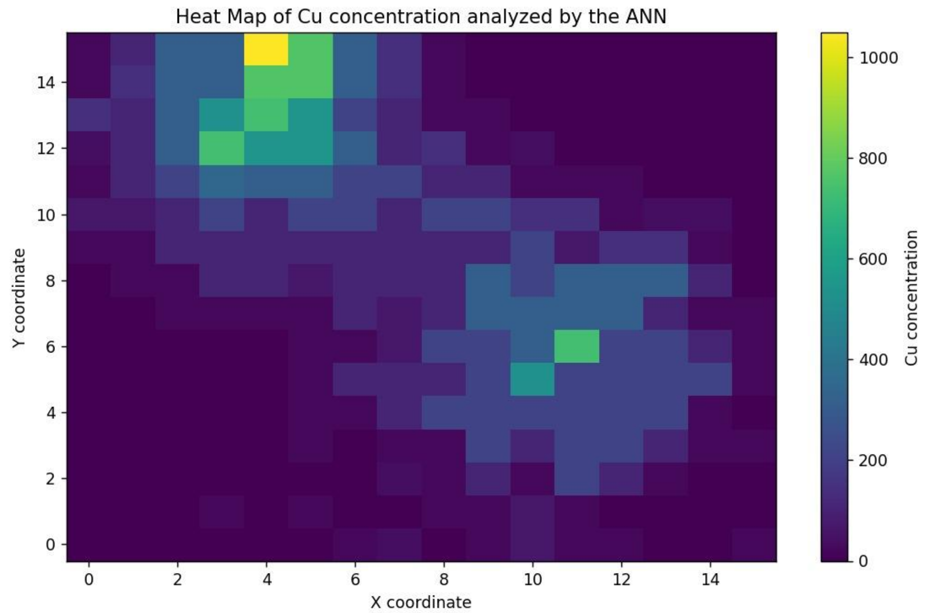
Ion beam analytical techniques (IBA) when recorded using a nuclear microprobe, allows to identify the elemental matrix of an unknown sample and to visualize the elemental distribution in 2D maps, and if Rutherford Backscattering Spectrometry (RBS) technique is used it is possible to obtain the depth profile of those elements. Using OMDAQ software, each scanned area is acquired as a 256x256 pixel map, each pixel containing all the IBA spectra recorded during the experiment.
A step forward in 3D imaging would be to represent the elemental depth profiling obtained in each pixel of the map. This means to analyse hundreds of RBS spectra, requiring time and computing resources. To tackle this problem we are developing an artificial neural network (ANNs) models, which once trained, can handle the analysis of large data sets instantaneously [1]. The potential of ANNs to automatically render depth profiles of several types of samples in a 3D environment will definitely extend the imaging capabilities of nuclear microprobes.
Herein we will report on an ANNs method to perform an automated analysis and classification of RBS spectra recorded during nuclear microscopy analysis of cells exposed to Cu complexes [2]. Challenges as the low statistics of the RBS spectra, the estimated time requirements for training the ANNs, or the visualization of the results will be presented and discussed.



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Exploring Deep Eutectic Solvents in Palladium Environmental Analysis: A First Look

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Palladium is a technology-critical element from the platinum-group with a variety of applications Yet, it is mainly used in catalytic converters of cars and industries. Thus, its concentrations have been increasing in several environmental compartments, including in the aquatic media and robust analytical methods are still needed for its quantification. The major analytical challenges on Pd determination are the high limits of detection (LOD) and interferences during the analysis of environmental samples. In this sense, Ni is the major interfering element when using voltammetry, whereas for inductively coupled plasma (ICP) methods several polyatomic and spectral interferences need to be controlled. A new generation of solvents named Deep Eutectic Solvents (DES), resulting from a Hydrogen Bond Donor (HBD) and a Hydrogen Bond Acceptor (HBA) mixed until liquid, has emerged as a green alternative for trace element analysis and recovery, owing to their excellent features. In this work, we used a DES selective for Pd for investigating the solvent applicability in Pd voltammetric analysis. The DES was composed by methyltrioctylammonium chloride ($N_{8881}Cl$ / Aliquat 366) as HBA and hexanoic acid as HBD in two different ratios, 0.23: 0.77 (DES_1) and 0.333: 0.667 (DES_3) [1]. Batch experiments were performed in 0.1 M HCl and synthetic seawater using:
i) 10 µL of each DES; ii) DES+100 µg/L Pd; and iii) DES+100 µg/L Pd+500 µg/L Ni, as schematized in Figure 1. Analysis of Pd and Ni were performed using square wave voltammetry, with limits of detection of 0.2 µg/L Pd using the DES.

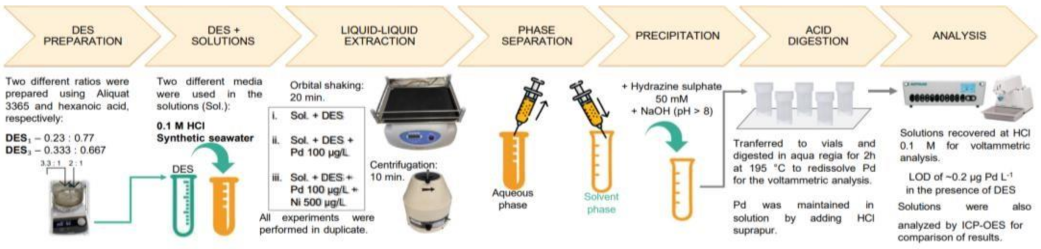

Figure 1. Scheme of the steps of the experiment, from DES preparation until the voltametric analysis.

In the aqueous phase, no signal of Pd was detected in all experimental conditions. Thus, the estimated extraction efficacy (%) of DES toward Pd was 99.8%. However, the recovery of Pd in the solvent phase ranged between 60 and 100%. Conversely, the simultaneously monitoring of Ni in the experiment confirmed the high selectivity of the DES toward Pd, with Ni remaining in the aqueous phase. The data obtained for the solvent phase show that in average 82% of Pd is transferred into DES1, and 93% into DES3. This work paves the way for innovative approaches to sample preparation and improvement of the analytical determination of Pd in environmental samples, particularly in aqueous matrices.

Keywords: Environmental analysis, Green chemistry, Analytical improvements
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Pre-targeting bioorthogonal strategy for tethering photoactive BODIPY onto the plasma membrane of HER2+ gastric tumours

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Early diagnosis of gastric cancer is crucial for increasing the survival rate. However, current diagnostic methods such as endoscopic ultrasound combined with immunohistochemistry and fluorodeoxyglucose (FDG) positron emission tomography-computed (PET-CT) are limited in providing static information. They are also only suitable for certain types of gastric cancer. To complement these methods, optical imaging using fluorescent probes, such as BODIPYs conjugated with monoclonal antibodies (mAbs), can improve tumour contrast and selectivity. However, the conventional method of preparing fluorescently labelled immunoconjugates by modifying lysine residues can result in a complex mixture and loss of affinity to the corresponding receptor. To address this challenge, the in vivo bioorthogonal approach involving inverseelectron-demand Diels-Alder reactions (iEDDA) between monoclonal antibodies (mAbs) modified with trans-cyclooctene (TCO) and tetrazine (Tz) is presented as an alternative. This approach allows the development of imaging agents directly within the living system, eliminating the need for prior mAbs modification with the bioimaging agent. BODIPYs are highly stable fluorescent molecules suitable for cell imaging. The human epidermal growth factor receptor 2 (HER2) overexpression in gastric cancer has made it a valuable tumour biomarker and therapeutic target in clinical practice. We first synthesised BODIPYtetrazine and then utilized it with the HER2 antibody trastuzumab as pre-targeting imaging agents to target HER2 receptors in gastric tumours (**Figure 1.**). The study presents preclinical findings on the potential of a click approach for delivering a fluorescent probe to target HER2+ gastric tumours in vitro and in vivo.

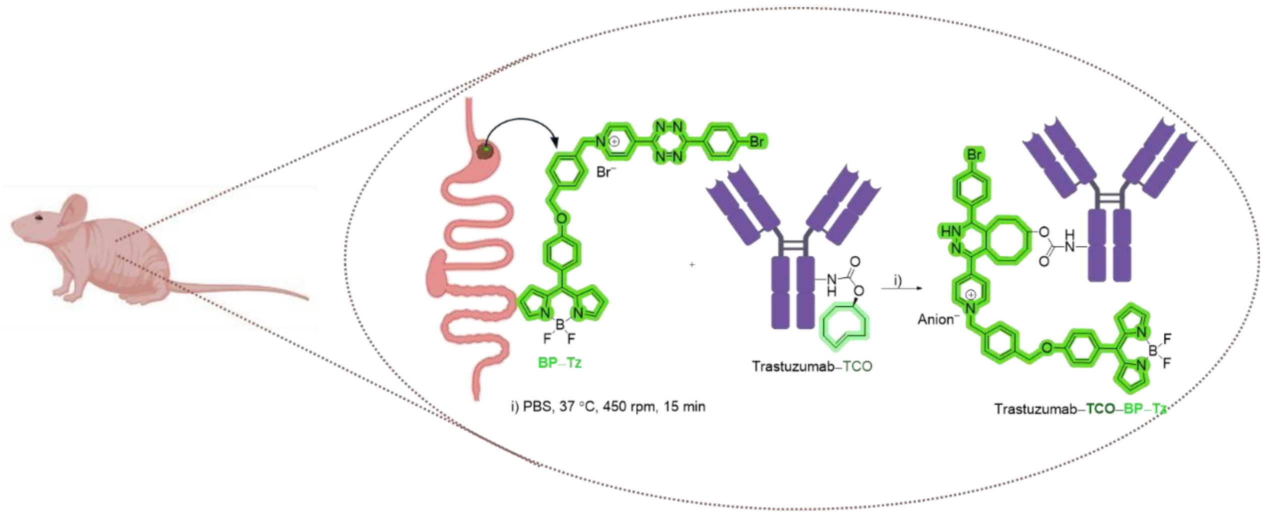

Figure 1. *In vivo* bioorthogonal approach with BODIPY-tetrazine.

Valorization of Arbutus unedo Bagasse using Eutectic Solvents for Cosmetic Applications

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The *Arbutus unedo*, also known as strawberry tree, is a small tree endemic to the Mediterranean region, and its fruits are rarely eaten fresh since they are only tasty when the fruit is fully ripped. Nevertheless, the strawberry tree fruit are usually consumed only after being processed into jams, sweets and alcoholic beverages. [1,2]

In the southern region of Portugal, the fruits are utilized to produce the traditional alcoholic liquor "Aguargente de Medronho". The liquor is made by distilling the fermented fruits, which results in an accumulation of leftovers that are typically thrown away. This residue, also known as bagasse, is considered a problem for the environment and the industry.[2] Despite the lack of research and characterization of this residue, the fruit has a well-known composition. Many researchers have pointed out the existence of bioactive substances that exhibit antioxidant activity, such as phenolic acids, flavonoids and polyphenols. These compounds may still be found in the residue since they are non-volatile.[3] These compounds with high antioxidant activity have several applications in different industries such as the pharmaceutical, food and cosmetics.[3]

The purpose of this research is to extract the phenolic and flavonoid compounds that are present in strawberry tree bagasse using natural deep eutectic solvents (NADES) to develop a cosmetic formulation with antioxidant properties. Strawberry tree fruit bagasse produced from two different regions from Portugal (Monsato and Viana do Castelo) were studied with the aim of comparing the phenolic and flavonoid contents as well as the antioxidant activity of the produced extracts. The total phenolic content, total flavonoid content, and antioxidant activity of strawberry tree residues were measured by colorimetric analysis of the extracts. As extraction solvents, proline and betaine based NADESs in combination with citric acid, propylene glycol and sugars were studied. During the NADESs screening process, the European Regulation for Cosmetics was followed. [4] Design of experiments was used in the optimization of the extraction conditions to improve the extraction yields. Additionally, pressurized liquid extraction was also studied, with the objective of understanding the potential impact of the techniques on the extraction of the target compounds.

As a proof of concept, water-in-oil formulations incorporated with the obtained extract were produced, and their rheological characteristics were analysed and studied.

Keywords: Strawberry tree bagasse, natural deep eutectic solvents, phenolic compounds, cosmetics, pressurized liquid extraction

Acknowledgments:
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Supercritical antisolvent microencapsulation of oil extract from microalgae *Cryphtecodinium cohnii*

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The increasing global population, along with the consequences of a progressing climate change have led to intense research for sustainable, environment friendly and efficient products in the various sectors of production and economy. Diverse bio-products, such as biofuels and biopharmaceuticals, are then ascending from a variety of natural sources.

Microalgae are unicellular or multicellular organisms, which have been been studied as a sustainable source for various bio-products due to their interesting characteristics. Pigments such as carotenoids, omega-3 fatty acids, sterols, enzymes and many others, with several health benefits, have been discovered, and the interest in these compounds lead to a possibility for a higher scale production.

Microalgae oils can present an alternative to terrestrial produced oil, such as vegetable oils, relieving the pressure on land use due to agricultural crops. However, these oils contain several compounds, such as carotenoids and polyunsaturated omega-3 fatty acids, that are very fragile to mechanical and thermal processes and can be easily degraded by alterations in the environment particularly when exposed to light, pH alterations, oxygen or air and high temperatures. In order for the microalgae oil to be used as high quality compound in industrial applications, these compounds need to gain stability and increase their bioavailability.

Microencapsulation processes can help to achieve these desired characteristics. In these processes a coating material surrounds the core substance that is the active ingredient of choice encapsulating it against the outside environment that could potentially degrade it.

The use of supercritical fluid technology as encapsulation technique can be considered a suitable green alternative, particularly interesting to process low soluble compounds.

The aim of this work was to study the use of the Supercritical Antisolvent micronization process (SAS) to encapsulate microalgae oil. Polyvinylpyrrolidone (PVP): K30 and K700, was used as a carrier material and different oil:PVP ratios were evaluated, being 1:1 the one with the higher concentration of oil in the starting mixture. The solvent used was a solution mixture of acetone and ethanol (2% v/v). The experimental parameters: pressure, temperature and flow rate of the solvent solutions were studied in ranges of 100 to 180 bar, 40 to 60 ºC and 0,5 to 1 mL/min, respectively, to evaluate their impact on the resulting particles. SEM analysis was used to evaluate the morphology of the micronized particles showing sub-micron spherelike particles which tended to aggregate. Particle size was measured through Dynamic Light Scattering, showcasing sizes ranging from 0,2 to 3 µm. FTIR analysis allowed for a characterization of the composition of the samples, that proved that a small quantity of oil was successfully encapsulated in the process. Differential Scanning Calorimetry (DSC) allowed to assess the composition of the precipitated material, that indicated a very similar heat flow profile to the PVP carrier material.

The results showed that high pressure and high temperatures (150 bar and 60ºC) lead to high micronization yield and the PVP K700 allowed to attain the highest micronization yield (60%). Lower pressures and high temperatures (100 bar and 60ºC) showed higher concentrations of oil in the encapsulates resulting in better efficiency of encapsulation but a lower yield (20%).

Keywords: Supercritical Antisolvent; SAS; Microalgae oil; Micronization; Polyvinylpyrrolidone

Acknowledgments: Centro de Química Estrutural is a Research Unit funded by FCT through projects UIDB/00100/2020 (https://doi.org/10.54499/UIDB/00100/2020) and UIDP/00100/2020 (https://doi.org/10.54499/UIDP/00100/2020). Institute of Molecular Sciences is an Associate Laboratory funded by FCT through project LA/P/0056/2020 (https://doi.org/10.54499/LA/P/0056/2020).

Photoinduced Plasmon-assisted Functionalization of Gold Nanorods for Improved Plasmon-based Sensors

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The strong interaction of gold nanoparticles with light, through collective oscillations of free electrons in the metal, has been explored in many ways to develop optical detection schemes for biochemical sensors. Generally, the detection scheme requires that target species interact with the particle's surface, which is accomplished by its modification with molecular recognition units. The motivation behind the development of regioselective functionalization strategies, as opposed to indiscriminate full surface coating, is based on a more rationale use of the particle's surface by directing the target species to its more sensitive regions (plasmon hot spots), while leaving other regions available for complementary functionalities, such as colloidal stabilization or anti-fouling coatings. The pursuit of such strategies has contributed to enhance single-molecule detection of proteins,1 and to the development of brighter fluorescent nanoprobes.2 Recently, we have explored a new photoinduced plasmon-assisted strategy to target hot spots in gold nanorods for modification with bioreceptor units. The biotin-functionalized gold nanorods respond specifically to streptavidin binding, thus, providing a model plasmonic biosensor with a total peak wavelength shift of ca. 4 nm (Fig. 1).

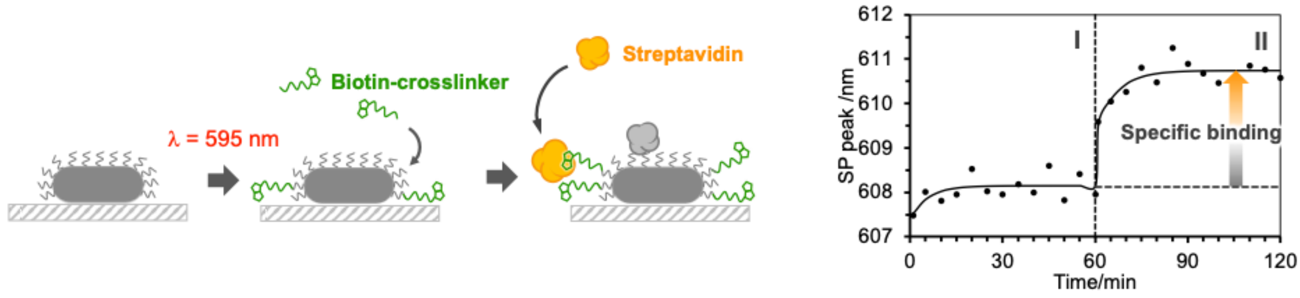

Figure 1. (Left) Functionalization of gold nanorods with biotin receptors using irradiation at surface plasmon (SP) resonance wavelength. (Right) Surface plasmon peak shift in response to streptavidin (100 nM) in PBS buffer.

Keywords: Optical sensors; Biorecognition; Nanoplasmonics; Photochemistry; Molecular diagnostics.

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Fluxes of Mercury and Methylmercury in Thermokarst Lakes

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The evolving Arctic environment, characterized by the gradual thawing of permafrost and the subsequent creation of thermokarst lakes, has promoted the remobilization of previously stored mercury (Hg), nutrients, and organic matter (OM) within the different environmental compartments [1]. These lakes provide favorable (anaerobic, OM and nutrient rich) conditions for methylating bacteria to thrive, leading to the formation of monomethylmercury (MMHg), the most harmful form of Hg, associated with high bioaccumulation/biomagnification rates and severe neurological effects [3]. This work focuses on quantifying the fluxes of Hg and MMHg between the bottom sediment layer and the overlaying water column in thermokarst lakes, which occur across the sediment/water interface (SWI) by means of various transport mechanisms.

Water samples were collected in summer 2024 from a thermokarst lake (SAS 1A) and a reference (bedrock) lake (K9) located in the Canadian sub-Arctic region Kuujjuarapik, using an in-*situ* benthic flux chamber (BFC). The concentration of Hg and MMHg in the samples were determined using CV-ICP-MS and GC-ICP-MS, respectively. In addition, the concentrations of other analytes — divalent iron (Fe^{2+}), total iron (Fe(T)), total manganese (Mn(T)), dissolved organic carbon (DOC), chloride (Cl^-), sulfate (SO_4^{2-}), nitrate (NO_3^-), ammonium (NH_4^+) and total sulfide (S^{2-}(T)) — were quantified using appropriate analytical techniques to better understand the Hg dynamics in these systems. The flux calculations for all analytes across the SWI were performed following the methodology proposed by Covelli *et al.* (2010) [3].

A preliminary analysis of the results indicated that the fluxes of Total Hg (THg) were generally negative (flowing from the water column to the sediment layer) in both lakes. Similarly, the fluxes of MMHg were predominantly negative; however, some anomalies showed positive fluxes during certain time intervals. Overall, high THg concentrations were found in SAS 1A (up to 6.0 ng L^{-1}), while MMHg levels were higher in K9 (range between 0.32 and 0,84 ng L^{-1}), with proportions of MMHg from THg (%MMHg) up to 38%. A more comprehensive analysis that incorporates all the previously mentioned analytes is currently in progress.

This study highlights that thermokarst lakes are particularly dynamic environments concerning the mercury cycle. Evaluating whether the bottom sediments in these lakes act as sink or source of Hg and MMHg to the water column is crucial, as they pose serious risk to consumers that rely on these aquatic systems for their survival, as well as to organisms at higher trophic levels.

Keywords: Permafrost, Thermokarst Lakes, Mercury, Monomethylmercury, Benthic Fluxes.

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Impregnation of soft contact lenses using supercritical fluids

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Abstract

Soft contact lenses (SCLs) have attracted increasing attention in the field of ocular drug delivery systems, owing to their potential to improve drug bioavailability in ocular tissues. However, the incorporation of some lipophilic drugs, in particular triamcinolone acetonide (TA), in these devices constitutes a significant challenge through conventional soaking methods. Supercritical carbon dioxide ($SCCO_2$) has emerged as a green-solvent alternative for the development of such delivery systems since it guarantees a solvent-free final product where poorly soluble drugs can be easily impregnated without the need for organic solvents. In this work, $SCCO_2$ impregnations (SCI) were conducted in a batch mode to improve drug loading from silicon-based contact lenses materials. First a silicone-based hydrogel (TRIS/NVP/HEMA, 40:40:20 w/w) was synthesised by thermal polymerisation at 60ºC for 24 h. Design of experiments was applied with the aim of screening the most significant experimental parameters on the TA SCI in the SCLs, as well as predicting the experimental conditions for maximum SCI. As so, a full factorial design at 4 factors, namely pressure (200 - 300 bar), temperature (40 - 60ºC), impregnation processing time (2 - 6 h) and presence of co-solvent (DMSO: 0 - 5% v/v) and at one response: yield of impregnation (i.e., TA SC loading of the produced SCLs materials) was performed. Impregnation yield was assessed through TA-release studies from the loaded SCLs. Also, an extensive characterisation of the material key functional properties for the conventional and SCI SCLs was carried out (e.g. transmittance, water content, mechanical properties, wettability, biocompatibility). Moreover, in vitro TA release studies were performed in skin conditions. The results demonstrated that TA-loaded SCLs materials can be successfully prepared using the employed SCI process. The highest impregnation yields were obtained with materials processed under the conditions of 300 bar and 60ºC, reaching the highest TA amount released (10.121 ± 0.44 µg/mg), which represents a 162.2% increase compared to the conventional loading process. The analysed properties showed that the produced materials were suitable for the intended application. The efficiency of the SCI process was demonstrated, but it was also evident the versatility of improving it by adjusting the conditions.

Keywords: Supercritical carbon dioxide, impregnation, drug loading, triamcinolone acetonide, soft contact lenses materials, drug delivery systems, drug-eluting contact lenses

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Determining the rhizosphere influence of *Halimione portulacoides* on mercury concentration and bacterial diversity in the saltmarsh sediments of the Tagus Estuary (Lisbon)

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Tagus Estuary is known to contain high levels of mercury (Hg), due to past industry activities. Given the high microbial activity observed in saltmarsh ecosystems and the pivotal role of plant-bacteria interactions in Hg cycling in the Tagus Estuary[1], this study evaluates the seasonal influence and the impact of *H. portulacoides* on the mercury content and bacterial communities of rhizosphere sediments.

Vegetated sediment and root samples were collected, in winter and spring seasons, in an area colonized by *H. portulacoides* and compared with sediments without plants. Mercury and methylmercury (MeHg) were quantified in vegetated (rhizosphere) and non-vegetated sediments and in *H. portulacoides* roots. Cultivation of aerobic, heterotrophic bacteria from vegetated and non-vegetated sediments was conducted for quantification of Colony Forming Units (CFU)/g. From these cultures 59 aerobic bacteria were isolated, tested for inorganic mercury (Hg^{2+}) resistance, and identified through 16S rRNA gene sequencing.

Results in sediments and roots showed high values, with contents of Hg and MeHg above normal values for unpolluted soil and water[2]. Concentrations of Hg and MeHg ranged from (0,130 ± 0,015) µg/g to (3,121 ± 0,108) µg/g and from (0,8 ± 0,02) ng/g to (27 ± 1) ng/g, respectively. In terms of CFUs/g, spring stood out with higher numbers, which might indicate the influence of temperature in bacterial abundance. Halotolerant, typical saltmarsh bacteria, such as *Vibrio spartinae*, were isolated from the rhizosphere of *H. portulacoides*. Regarding mercury resistance, a clear difference was identified, with a higher percentage of rhizosphere bacteria presenting signs of resistance, some of which affiliated with the genera *Vibrio* and *Microbulbifer*, compared to unvegetated sediment bacteria.

In conclusion, this study reveals higher MeHg content in plant roots than in rhizosphere and bulk sediments, suggesting that areas colonized by *H. portulacoides* may be hotspots for the recruitment of Hg-methylating bacteria in saltmarsh ecosystems.

The authors acknowledge funding by Fundação para a Ciência e Tecnologia (FCT) through the UIDB/04565/2020 and UIDP/04565/2020 projects awarded to iBB and Centro de Química Estrutural, Instituto Superior Técnico (CQE-IST) through projects UIDB/00100/2020 and UIDP/00100/2020, This work was also funded by the 'Blue Bioeconomy Pact' (Project no. C644915664 00000026), co-financed by the European Fund's 'Next Generation EU'. AMF is the recipient of a PhD grant [BL99/2024] funded by project no. C644915664-00000026. Rute Cesário is funded by National funds (OE) through FCT under the Scientific Employment Stimulus–Individual Call 2021.03267.CEECIND/CP1651/CT0010.

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Effect of Plants on Mercury Dynamics in Permafrost Thaw Systems

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The Minamata Convention on Mercury has recognized mercury (Hg) as a chemical of global concern [1]. Of particular importance is methylmercury (MeHg), the most stable and toxic organic form of mercury, known for its strong neurotoxic effects [2]. Recent research suggest that Arctic permafrost is a large global reservoir of Hg [3], which is vulnerable to degradation under a warming climate, presenting a new threat to the northern ecosystem. Therefore, the main goal of this study is to evaluate the contribution of plants to the mercury budget in the context of permafrost degradation.

Vegetated and non-vegetated sediment cores and aerial plant parts were collected from the shores of two lakes in the Canadian subarctic (Nunavik, Quebec): a permafrost thaw lake designated as SAS-1A and a bedrock lake designated as K9. In this study, it was used stable isotope tracers of ^{200}Hg and $MM^{198}Hg$ followed by isotope-specific detection with inductively coupled plasma mass spectrometry. This approach enabled the determination of methylation rates in the vegetated and non-vegetated samples as well as ambient concentrations of total Hg (THg) and MeHg.

Results showed higher concentrations of ambient THg and MeHg in lake K9, in sediments colonized by mosses, respectively, 624 ng g^{-1} and 87.8 ng g^{-1}. In opposite, lowest ambient Hg and MeHg concentrations were found in non-vegetated sediments in lake K9 (ranging from 5 to 17.6 ng g^{-1} for THg and from 0.08 to 0.46 ng g^{-1} for MeHg). In lake SAS-1A, concentrations of THg and MeHg were up to 175 ng g^{-1} and 7.89 ng g^{-1}, respectively. Furthermore, the highest methylation rate (20.03 %) was also observed in lake K9 in sediments colonized by mosses.

In conclusion, results demonstrate that the presence of plants, especially mosses, enhances MeHg formation, shown by higher methylation rates in vegetated sediments compared to non-vegetated sediments.

The authors acknowledge the Portuguese national funds provided by Fundação para a Ciência Tecnologia (FCT) through the projects THAWPLANT (funded by Portuguese Polar Program-PROPOLAR) and Centro de Química Estrutural, Instituto Superior Técnico (CQE-IST) projects UIDB/00100/2020 and UIDP/00100/2020, Rute Cesário is funded by National funds (OE) through FCT under the Scientific Employment Stimulus–Individual Call 2021.03267.CEECIND/CP1651/CT0010

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Spatio-temporal assessment of variations in mercury levels in saltmarsh regions of the Tagus and Guadiana estuaries

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Mercury (Hg) dynamics in estuarine sediments have been extensively studied, yet the processes driving temporal changes in mercury concentrations and speciation remain less understood in historically contaminated regions. The Tagus estuary has been impacted by anthropogenic Hg inputs, particularly in Barreiro, Cala Norte and Alcochete, while Castro Marim area, in the Guadiana estuary, is naturally influenced by the nearby pyrite belt and serves as a reference site. This study investigates the spatial and temporal distribution of total mercury (THg) and monomethyl mercury (MMHg) concentrations in sediment cores from these regions, with a focus on identifying historical trends and the current status of mercury cycling.

Sediment cores were analysed to quantify THg and MMHg concentrations, with MMHg/THg ratios calculated to assess methylation efficiency. Results show distinct patterns of mercury accumulation between vegetated and non-vegetated areas. In Alcochete, non-vegetated sediments showed higher MMHg concentrations, up to 3.27 ng/g, and THg levels, up to 0.71 µg/g, while vegetated areas exhibited lower Hg concentrations. The MMHg/THg ratios indicated more efficient methylation in surface layers, decreasing with depth. In Barreiro and Cala Norte, similar trends were observed, with vegetated sites generally exhibiting higher MMHg concentrations and MMHg/THg ratios than non-vegetated areas, suggesting enhanced methylation in these environments. Conversely, non-vegetated areas showed more pronounced THg concentrations. Castro Marim exhibited lower overall Hg concentrations compared to Tagus sites, with MMHg levels up to 2.28 ng/g and THg up to 0.40 µg/g in the vegetated core.

Overall, the Tagus estuary exhibited higher mercury concentrations and more varied methylation patterns across its sites. In contrast, Castro Marim, despite lower overall mercury levels, still displayed evidence of ongoing methylation processes, particularly in vegetated sediments.

The authors acknowledge the Portuguese national funds provided by Fundação para a Ciência e a Tecnologia (FCT) through Centro de Química Estrutural, Instituto Superior Técnico (CQE-IST) projects UIDB/00100/2020 and UIDP/00100/2020, Rute Cesário is funded by National funds (OE) through FCT under the Scientific Employment Stimulus–Individual Call 2021.03267.CEECIND/CP1651/CT0010.

Experimental Wind Turbine Simulator

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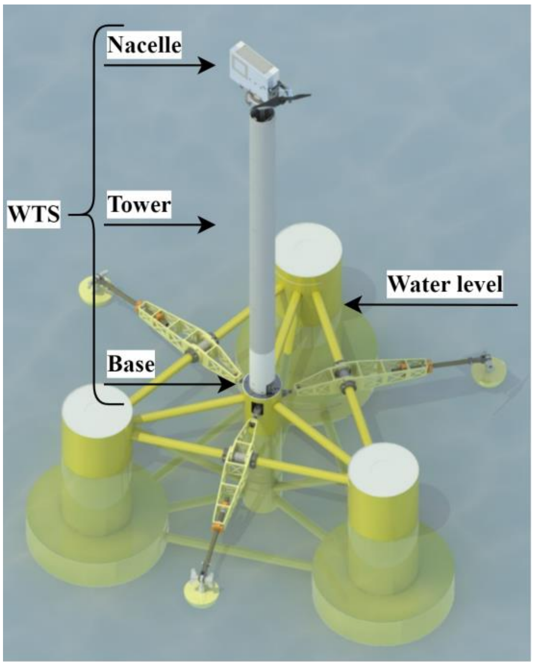
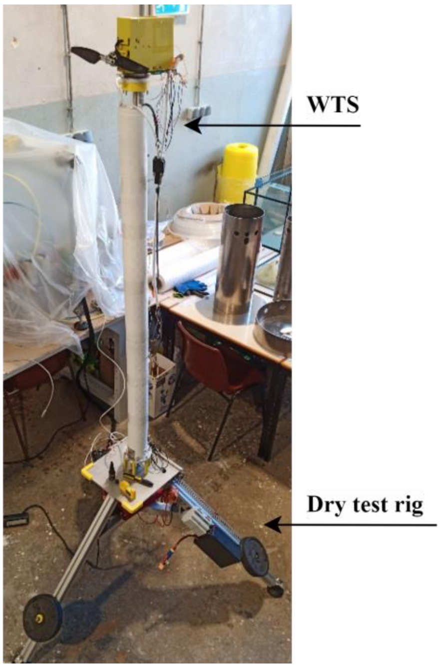
This poster presents an experimental Wind Turbine Simulator (WTS) for testing a Floating Wind-Wave Platform concept (FWWP). This concept aims to minimize cyclic loads on the wind tower and platform, induced by wind and waves, with severe fatigue damage on the tower base and top locations, such as blades, rotor shaft, yaw bearing, gearbox, and generator. The strategic objective of the concept is to reduce the cost of electricity produced from offshore renewable energies in the medium and long term by using higher power wind turbines. Thus, providing conditions for the commercialization of this technology.

The WTS simulates the physical thrust on the nacelle caused by the wind on the WT blades. This is achieved with the Hardware In the Loop simulation (HIL) approach that integrates the wind and blades' numerical models with the physical one (WTS). A load cell is installed at the WTS base to measure cyclic loads caused by thrust variations on the nacelle and inertial sensors are located inside the nacelle to measure motions and accelerations. These data are used to control platform motions and to evaluate the impact on FWWP structural integrity. The WTS prototype was designed and built by CENTEC and is currently under improvement. Then, further dry testing will be performed, before attaching the WTS to the floating platform model, for wet testing in a wave tank. The design and preliminary results are presented in this poster.





Keywords: Floating Wind-Wave Platforms, Structural Integrity, Hardware In the Loop Simulation, Dry Testing, Prototype Design.

Acknowledgments: This work was performed within the CENTEC Strategic Research Plan, which is financed by the Portuguese Foundation for Science and Technology (FCT) under contract UIDB/UIDP/00134/2020 and the project "Variable geometry Wave Energy Conversion system for floating platforms", financed by FCT and under contract PTDC/EME-REN/0242/2020. The equipment was built in collaboration with the NOF workshop (Núcleo de Oficinas) and the Laboratory of Naval Architecture and Ocean Engineering at Instituto Superior Técnico. The authors would like to thank their support.

Ion Beam Analytical techniques combined for the characterization of cultural heritage materials

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Cultural heritage materials analysis often require the use of non-destrutive analytical techniques. Analysis with MeV ion beams have that required capability together with high sensitivity with extended information obtained when combining different spectrometry techniques as PIXE (Particle Induced X-ray Emission), RBS/EBS (Rutherford/Elastic Backscattering Spectrometry), PIGE (Particle Induced Gamma-Ray Analysis), NRA (Nuclear ReactionAnalysis) and/or ionluminescence. With the use of a scanning nuclear microprobe lateral spatial information with micrometer resolution and imaging can be obtained. In this work are presented some case studies carried out at the Laboratory of Accelerators and Radiation Technologies from IST where the advantages of the combination of IBA techniques are explored and applied to the study of metal, ceramics, glass or manuscript samples.

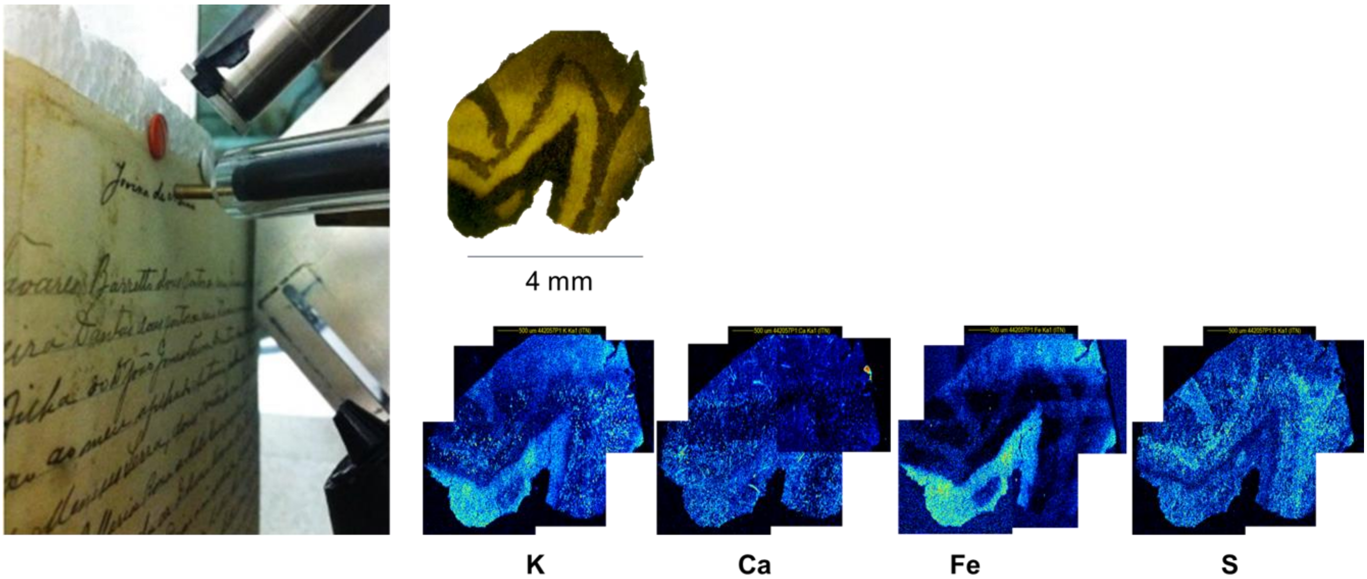

Figure 1: Elemental distribution maps for the characterization of a 17th century manuscript fragment written with iron-gall ink [1].

Keywords: Ion Beam Analysis, elemental distribution, elemental depth profile, Cultural Heritage materials.

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Microencapsulation of a Far-Red absorbing Phthalocyanine: recent advances on microscale engineering of polyelectrolyte multilayers

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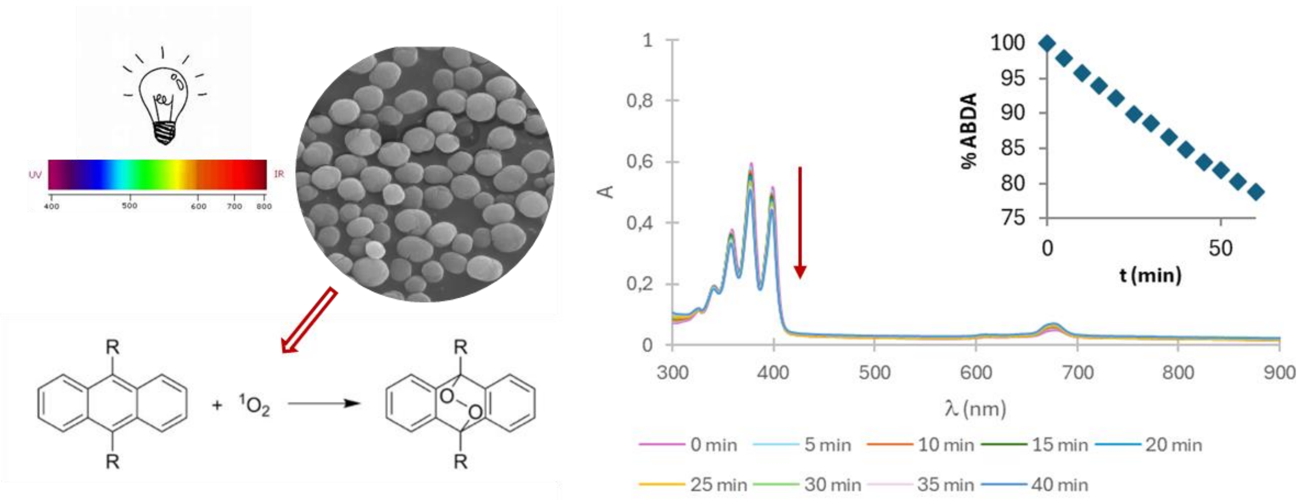
Polyelectrolyte microcapsules (PECs) have been created on Layer-by-Layer technology, by alternately layering of positive and negative charged polyelectrolytes on dispersed nano- or micro- particles. These systems have promising applications in drug delivering, biosensing, and as micro-reactors. They can integrate light-absorbing photosensitizers, such as porphyrins and related, enabling the creation of optically addressable devices. Herein we report recent advances regarding PECs design and functionalization aiming to improve light triggered processes across polyelectrolyte shells. It is shown that the rational assembly of cores, dyes and polyelectrolyte multilayers are the key parameters that rule pH-controlled porphyrin adsorption and release [1]. Further, PECs were also employed as micro reactors for the construction of needle like porphyrin J aggregates [2]. Recently, we have shown that PECs are valuable platforms towards the preparation of spectrally engineered microsystems for efficient plasmonic fluorescence enhancement of porphyrins [3]. As an extension of that work, and to explore the relevance of using far-red absorbing dyes, a tetrasulphonated aluminum phthalocyanine has been selected. Different encapsulation conditions have been tested to evaluate the effect on the photodynamic outcome.



Keywords: Phthalocyanine, Polyelectrolyte Microcapsules, singlet oxygen, gold nanoparticles.

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October 29 - Oral Sessions

Modelling Reflectometry Diagnostics:
Finite-Difference Time-Domain Simulation of Reflectometry in Fusion Plasmas

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Reflectometry simulations are particularly important since they permit to assess the measuring capabilities of existing experimental systems and to predict the performance of future ones. We present a brief overview of reflectometry together with a short introduction to the Finite Difference Time Domain (FDTD) method for the simulation of reflectometry. The goal is to prepare the listener for the presentation of the family of REFMUL* codes, which incorporate new numerical solutions such as new kernels and source techniques. Their use allows to set up synthetic diagnostics that not only consider the wave propagation in a given plasma, but also take into account the system's location within the vacuum vessel, together with a characterization of its access to the plasma (wave guides and antennas). The synthetic diagnostic is complemented with the signal processing techniques necessary to process the measured reflectometry data.

We illustrate the use of synthetic diagnostics in the assessment of the Plasma Position Reflectometers of ITER and DEMO.

Keywords: Reflectometry; Plasma Physics; FDTD; Computational electromagnetics; REFMUL*

Axions in plasmas and metamaterials

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Axions represent one of the most elegant and theoretically compelling extensions to the standard model. Though they have remained elusive thus far, they were originally proposed to address the apparent violation of charge-parity (CP) symmetry in QCD—commonly known as the strong CP problem—by transforming the small CP angle observed experimentally into a field. In this way, the axion dynamically restores CP symmetry in QCD, much like how the Higgs boson provides mass to gauge fields [1]. Additionally, the subtlety of this CP violation leads to an extremely weak interaction with photons, making axions a highly attractive dark matter candidate. As a result, the axion has become one of the most sought-after particles, with numerous experiments currently dedicated to its detection.
A key limitation of current experimental approaches is their reliance on axion-photon conversion, a non-resonant process [2]. A promising alternative involves the use of plasmas, which enable resonant axion-plasmon conversion. We demonstrate that harnessing the physics of electrostatic instabilities in plasmas can significantly boost the conversion probability—or axion decay rate—by several orders of magnitude [3]. Furthermore, by replacing real plasmas with synthetic (metamaterial) plasmas, it may become possible to explore the parameter space for axions predicted by QCD. Finally, given the ubiquity of plasmas in various astrophysical environments [4], we explore the implications of axion-plasmon conversion in axion production within magnetars and discuss its relevance in intergalactic plasma environments.

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New Operation and Collaborative Tools for Advancing ITER Neutral Beam Test Facility Research

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The ITER Neutral Beam Test Facility (NBTF) is an important testbed to the advancement of neutral beam injection system crucial for ITER's experimental fusion power plant. It conducts two key experimental campaigns: SPIDER and MITICA. SPIDER focuses on developing the negative ion source that will produce deuterium ions for ITER, employing a prototype approach to optimize ion generation and acceleration. MITICA complements this by demonstrating a full-scale neutral beam injection system designed for plasma heating and control in ITER. As SPIDER resumes operations in April 2024 after a major shutdown aiming at several machine improvements, its emphasis is on refining the negative ion beam characteristics, aiming for enhanced beam uniformity and operational efficiency.

Central to the NBTF's success are advanced operational tools based on the Experimental Physics and Industrial Control System (EPICS) and MDSplus, which facilitate real-time monitoring, data management, and collaboration among international researchers. The implementation of these tools supports effective data analysis and decision-making, fostering communication across diverse scientific communities in Europe, India, and Japan. The use of remote collaboration technologies enhances accessibility, allowing global experts to visualize data in real-time and engage in coordinated research efforts.

This contribution details the architecture and deployment of the operational instrumentation, developed using tools such as Grafana, Redis and Python, providing remote participation, data visualization, and efficient collaboration. The results showcase improved operational parameters, including an increased pulse repetition rate and enhanced system performance. Future developments will aim to expand these capabilities further, addressing complex experimental needs and ensuring the NBTF continues to meet the evolving demands of fusion research. Collaborative efforts among EUROfusion, ITER, and various stakeholders remain essential for driving innovation and sustaining alignment with the broader goals of fusion science.

Improved voltammetric method for detecting Pd and Ni simultaneously using signal transformation

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Palladium (Pd) is a technology-critical element raising environmental concern, even at trace levels. Its concentrations in aquatic media vary from 0.04 ng/L [1] up to 3.2 µg/L, the latter usually found in wastewaters [2]. Nickel (Ni) is a trace element essential for organisms, but high concentrations can have a negative impact. Moreover, it is also the main interferent in Pd determination by voltammetry. Concentrations of Ni in aquatic environments can range from 0.07 µg/L up to 2.6 µg/L [3], yet in wastewaters it can vary up to 16 µg/L [4]. Therefore, the aim of our study is to improve the analytical determination of Pd while monitoring Ni simultaneously, which can be done by a suitable choice of the medium pH taking advantage of Pd and Ni complexes with dimethylglyoxime (DMG) [5,6]. In addition, square wave voltammetry (SWV) was used to improve the sensitivity of the determination, with the second derivative signal transformation applied (Fig.1). The experimental conditions for the simultaneous determination of Pd and Ni were optimized in terms of electrolyte composition, in addition to the pH, frequency (Hz), deposition time (t_d) and deposition potential (E_d). By fixing Pd and Ni concentrations (1.5 and 10 µg/L, respectively), a reduction in the pH decreased only Ni signal. The increase of DMG concentration had no effect on Pd signal but increased the sensitivity of Ni. Therefore, Ni interference on Pd signal can be overcome by controlling the electrolyte composition. Additionally, the frequency (25 Hz) of SWV contributed to a better separation of Pd and Ni voltametric signals. Increasing the E_d to more negative values led to a loss of Pd signal and an increase of Ni, thus -0.2V was chosen. A linear increase of both metal signals with the t_d was also observed. The limit of detection (LOD) for Pd and Ni was 0.02 µg/L and 0.20 µg/L, respectively. The improved method was applied to environmental matrices and certified materials.

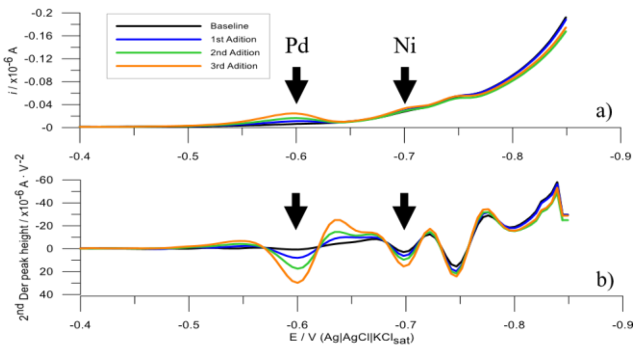

Fig. 1 – Original (a) and second derivative (b) voltamograms for Pd and Ni.

Keywords: Palladium, Nickel, Square Wave Voltammetry, Second Derivative Signal Transformation

Acknowledgements: The authors acknowledge FCT for funding projects SPECS (https://doi.org/10.54499/2022.06832.PTDC); CQE (https://doi.org/10.54499/UIDB/00100/2020 and https://doi.org/10.54499/UIDP/00100/2020); and the Associate Laboratory Institute of Molecular Sciences (https://doi.org/10.54499/LA/P/0056/2020).

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DNA Origami Tetrahedra for Positioning of Plasmonic Gold Nanorods Antennas

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The light manipulation achieved by plasmonic nanoparticles (NPs) has been leveraged in the design of several optical biosensors. In particular, emission enhancement of fluorophores by localized surface plasmon resonance (LSPR) carries potential in allowing for single-molecule detection through intensification of the signal given by reporter dyes, and could therefore be used to improve detection of very low concentration analytes. LSPR are localized resonant oscillations of a NP's electron cloud, resulting from interactions with an incident light of a particular wavelength, dependent on the NP's properties. LSPR leads to the enhancement of the electric fields in the immediate vicinity of the NPs surface, which can intensify the emission of a fluorophore contained in these fields. Further intensification is possible by coupling the electric fields of multiple NPs in close proximity, resulting in plasmonic "hotspots" between them. Of the several methods available to position these plasmonic nanoparticles, DNA origami is likely the most accessible. In this nanofabrication method, a long ssDNA scaffold is folded into a defined 3D shape by the concerted action of several small oligos called staples. We have designed and constructed a tetrahedral origami nanostructure to serve as the foundation of a novel biosensor for ssDNA/RNA biomarkers, that seeks to use plasmonic gold nanorods (AuNRs) to enhance the emission of a reporter dye for single-molecule detection. The origami is designed to position a AuNR dimer pointing towards the centre of the tetrahedra, forming a plasmonic "hotspot" at its centre. A capture ssDNA strand is positioned inside this hotspot to allow the sequential immobilization of the nucleotide biomarker, followed by a imager strand functionalized with a reporter dye. The origamis design was examined through *in silico* molecular dynamics simulations, using the oxDNA coarse-grained model, and was successfully constructed, as validated through agarose gel electrophoresis and fluorescence correlation spectroscopy (FCS). We have conducted preliminary studies of the DNA origami nanostructure without NRs through fluorescence microscopy and are currently attempting hybridization of the tetrahedra and NRs.

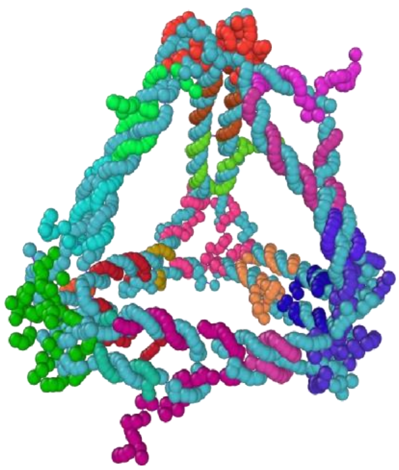

Figure 1. Molecular dynamics snapshot of DNA nanotetrahedron.

Keywords: Nanoplasmonics; DNA nanostructures; Biosensors; Nanorods;

Distribution Patterns and High-Concentration Areas of Metal Pollution in Soils from Fildes Peninsula, King George Island, Antarctica

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Previous studies have highlighted environmental contamination by major and trace elements in Antarctica, besides several organic contaminants linking to human activities. The ReACT project capitalizes on these studies and envisages the application of a site-specific, adjusted to the extreme conditions in place, Ecological Risk Assessment (ERA) Framework to the Fildes Peninsula, King George Island. Comprehensive analysis of the ecotoxicological Line of Evidence (EcotoxLoE) highlighted several sites bearing potential ecological risk, two of them being consistently signalled by all the organisms tested as those yielding the highest toxic potential. In this work, the objective was to explore the cause for this ecotoxicological hazard by developing on the chemical LoE of the ReACT ERA. Therefore, the same 20 soil samples collected in Fildes Peninsula (plus two likely reference areas in Ardley Island and Nelson Island) for the Ecotox LoE were analyzed for their burden in trace elements potentially toxic to the biota: Cr, Ni, Cu, Zn, As Cd, Pb and Hg. The bioavailability of these elements was also addressed by quantifying the leached fraction in naturalistic extractions with water (soil eluates). Total contents of Pb, Ni and Cu in soils were lower than the baseline values1 but in the same order of magnitude, although, Zn and Cd concentrations were 8 and 3 times higher. Additionally, Hg (3.6-21.6 ng/g) and As (3.9-122 µg/g) were the most concerning cases with concentrations of 31 and 12 orders of magnitude higher, respectively, than the previously reported. Surprisingly, the relatively high organic matter content (> 6%) indicated low mineralization rate, at least in some points, suggesting low leaching of contaminants, also observed by the low concentrations of trace elements in soil eluates, and consequently their low bioavailability to biota. In spite of the low potential bioavailability observed, elevated As and Hg levels found are concerning and can link to the effects denoted by previous ecotoxicological tests.

Keywords: Metal contamination; Ecotoxicology; Risk assessment; Antarctida.

References:

1- Lu, Z., Cai, M., Wang, J. et al. Baseline values for metals in soils on Fildes Peninsula, King George Island, Antarctica: the extent of anthropogenic pollution. Environ Monit Assess,184, 7013–7021 (2012). https://doi.org/10.1007/s10661-011-2476-x

2- Vítězslav Vlček, David Juřička, Jitka Míková. Heavy metal concentration in selected soils and sediments of Livingston Island, Deception Island, King George Island, James Ross Island (Antarctica), CZECH POLAR REPORTS 7 (1): 18-33, 2017, DOI: 10.5817/CPR2017-1-3

October 29 - Round Table

TUESDAY OCTOBER 29th 15h - 17h

NInTec Science Days 2024 addresses science policy issues in parallel with the main scientific program.

This second edition will focus on the

"Evaluation Methods for Researchers and Research Assessment"

The event promoted a round table in this topic, including a panel of invited speakers and the participation of the audience.

MODERADORA

Doutora Dulce Belo, Investigadora Principal do Departamento de Engenharia Ciências Nucleares, Membro da Direcção do NInTec

Bio

CONVIDADA

Professora Cecília Rodrigues, Vice-Reitora da Universidade de Lisboa

Bio

CONVIDADO

Professor Miguel Ayala Botto, Vice-Presidente do Conselho Científico do IST

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CONVIDADO

Doutor Bruno Béu, Assessor do Conselho Directivo da FCT

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