

## **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.

NInTec is pleased to present the first 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.

**NINTec Science Days** will also address science policy issues in parallel with the main scientific program. In this first edition, it will be discussed "The scientific employment: from University to the private sector". The event will promote a round table, including a panel of invited speakers and the participation of the audience.

NInTec acknowledges the support from <u>Impersol</u>, Hugo O'Neill (Graphic Designer), <u>SarsSpec</u> and <u>Instituto Superior Técnico.</u>

More information about the event can be found <u>here</u>.





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## Scientific Programme

## Thursday, October 6

10:00 - 10:20 Opening Session with Dulce Belo (NInTec President) and Rogério Colaço (Técnico President)

#### 10:20 - 11:20 First Scientific Session - Chair Dulce Belo

- 10:20 AM Nuno Canha Oxidative potential of fine aerosols from a Portuguese urban-industrial area
- 10:40 AM João Avó Nanomaterials with thermally-activated delayed fluorescence for sensing and imaging: challenges and solutions
- 11:00 AM Joana Madureira Valorization of olive wastes to develop food bioactives using ionizing radiation

#### 11:20 - 11:40 Coffee Break

#### 11:40 - 13:00 Second Scientific Session - Chair Leonor Maria

- 11:40 AM Victoria Corregidor Nuclear Microprobe: The Tool to Characterize Materials
- 12:00 PM Sandra Rabaça Conducting bilayer salts (CNB-EDT-TTF)4A
- 12:20 PM Joana Santos Novel Radioconjugates for Auger Electron Therapy of Prostate Cancer
- 12:40 PM Euripides J. Sellountos Hyperisingular Boundary Element Methods (BEM) in Navier-Stokes equations

#### 13:00 - 14:00 Lunch Break

#### 14:00 - 15:00 Third Scientific Session - Chair Jónatas Valença

- 2:00 PM Mário Rui Arruda New Fireproof Dwellings for Wildfire
- 2:20 PM João Canário The role of volcanism as a source of trace elements to the environment: The case of Deception Island Antarctica
- 2:40 PM Maria Eugénia Leitão Conceptualizing Socio-Tech Entrepreneurship
- 15:00 16:00 Scientific Poster Session with Coffee Break service

#### 16:00 - 17:00 Fourth Scientific Session - Chair Victoria Corregidor

- 4:00 PM Hugo Terças Plasmonic Instabilities in two-dimensional Dirac Materials
- 4:20 PM Rodrigo Mateus Ion beam analysis of Li-Sn alloys
- 4:40 PM Rogério Jorge Optimization of Alpha Particle Confinement in Fusion Devices



#### 17:00 - 18:00 Fifth Scientific Session - Chair Hugo Terças

- 5:00 PM Maria Catarina Carreira Influence of culture media on Mesenchymal Stromal Cell expansion and hematopoietic support capacity
- 5:20 PM Ana Fernandes-Platzgummer Manufacturing cultured meat through a scalable and cost effective bioprocess
- 5:40 PM Jorge João Purification of small heat shock protein nanocages: exploring a chromatographic approach

#### Friday, October 7

#### 09:20 - 10:40 Sixth Scientific Session - Chair Nuno Cruz

- 9:20 AM Pedro M. R. Paulo Bringing light closer to molecules for a sensitive detection of disease biomarkers
- 9:40 AM Rui Oliveira-Silva A single-particle plasmon sensor to monitor proteolytic activity in real-time.
- 10:00 AM Luis Nobre Supercritical antisolvent precipitation: a path to nanocatalysts.
- 10:20 AM Pedro Santos Novel bio-based Gold nanoplatforms for cancer phototherapy

#### 10:40 - 11:00 Coffee Break

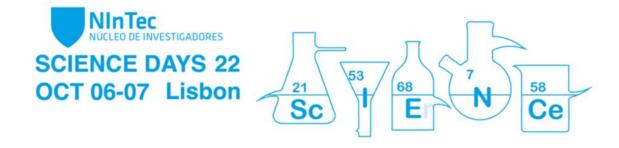
#### 11:00 - 12:40 Seventh Scientific Session - Chair Pedro Paulo

- 11:00 AM Nuno Cruz High-performance instrumentation for diagnostics and control in fusion devices
- 11:20 AM Pedro Santos Radiation for Material, Environmental and Health Sciences Research at IRIS
- 11:40 AM Nuno Veiga Fleet of drones for radiological inspection, communication, and rescue
- 12:00 PM Gonçalo Dias From Gravity to Gravity Waves: a Cursus Honorum
- 12:20 PM Emmanuel Zambrini Cruzeiro Quantum correlations: from quantum mechanical foundations to applications

12:40 - 14:30 Lunch Break

14:30 - 17:00 Round Table - Chair/Moderator José Vicente





## October, 6 Oral Session



#### Oxidative potential of fine aerosols from a Portuguese urban-industrial area

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Oxidative potential (OP) of aerosols is considered as a highly relevant indicator to characterize the toxicity of particulate matter (PM), with recent studies associating OP measurements to adverse health effects. The dithiothreitol method (OP<sup>DTT</sup>) has been widely used to assess OP of particles and it has been linked to airway inflammation markers, cellular oxidative stress markers, cellular cytotoxicity and cardiorespiratory health endpoints in epidemiological studies. These results support OP as a highly health relevant air quality parameter. However, specific chemical species, aerosol sources and processes that affect the OP of PM are still not well established. Currently, no studies are available for Portugal.

Fine aerosols (PM2.5) were sampled during one year (Dec 2019-Nov 2020, total of 128 sampling days) in an urban-industrial area of the Metropolitan Area of Lisbon (Seixal, Portugal) and their chemical composition was assessed to perform a source apportionment study using Positive Matrix Factorisation. A total of 7 different sources were identified: soil, secondary sulphate, fuel-oil combustion, sea, vehicle nonexhaust, vehicle exhaust and industry. Thirty samples were chosen considering the highest load for each source (both massic or %), which could eventually allow to understand the impact of each source regarding its associated OP, assessed by the dithiothreitol (DTT) method. The final DTT activity of samples was normalised in terms of sampled air volume and in terms of collected aerosol mass.

Samples presented mean levels of DDT activity (normalized to the mass) of  $11.9 \pm 6.8$  pmol/min\*µg, ranging from 2.6 to 26.1 pmol/min\*µg. The DDT activity (normalized to the sampled volume) showed to have an association with the PM2.5 levels, as shown by Figure 1.

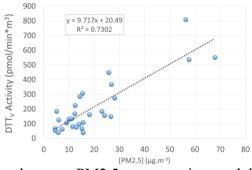


Figure 1. Correlation between PM2.5 concentrations and their DTTv activity.

Considering that the contribution in mass of the different sources was known to the PM2.5 levels, Spearman correlations were conducted and it was found significant correlations between DTTv and two different sources: vehicle exhaust (R2=0.651, p-value = 0.001) and fuel-oil combustion (R2=0.510, p-value = 0.016). Future work will assess the OP of the remaining samples to evaluate the contribution of the different sources for the OP of fine aerosols in the study area.

#### Acknowledgements

This work was supported by the Portuguese Foundation for Science and Technology (FCT, Portugal) through the project HypnosAir (PTDC/CTA-AMB/3263/2021), the contract 2021.00088.CEECIND (N. Canha) and the financial support to C2TN/IST (UIDB/04349/2020+UIDP/04349/2020). The COST Action CA17136 – Indoor Air Pollution Network is also acknowledged for supporting the Short Term Scientific Mission of N. Canha at DISTEBA (Lecce, Italy).

Keywords: fine aerosols; oxidative potential; urban areas; source apportionment; air pollution



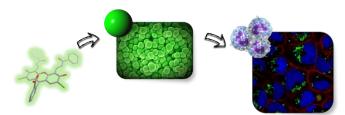
## Nanomaterials with thermally-activated delayed fluorescence for sensing and imaging: challenges and solutions

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Thermally activated delayed fluorescence (TADF) recently emerged as the most effective strategy to convert non-emissive triplet states in emissive excitons in OLEDs.<sup>1</sup> This luminescence usually displays lifetimes in the micro-to-millisecond timescale and is highly sensitive to external conditions, including polarity, temperature or oxygen concentration, which provides an ideal platform to develop optical probes timeresolved optical imaging or in sensing of local temperature or oxygen concentration in vivo.<sup>2</sup> However, TADF molecules perform poorly in polar media, and additional steps must be taken to enable their use in biological applications. Herein, we describe how nanoaggregation and nanoencapsulation of TADF emitters in silica and polymeric nanoparticles can be effective straightforward methods to achieve TADF emission in water with high luminescence quantum yields and remarkable delayed-to-prompt fluorescence ratios and discuss the advantages and disadvantages of the different approaches. Through careful selection of optical probes and nanocarrier matrix, it is also possible to tune luminescence lifetime and oxygen permeability for optimal oxygen sensitivity in physiological conditions, as well as achieve luminescent probes with excellent biocompatibility and cellular uptake and distribution for application in fluorescence microcopy imaging.<sup>3,4</sup>



*Figure.* A TADF emitter is grafted onto silica nanoparticles and used as a luminescent probe in fluorescence imaging of cancer cells.

**Keywords:** Luminescent organic dyes; Luminescent nanomaterials; Thermally-activated delayed fluorescence; Optical Spectroscopy; Fluorescence microscopy imaging.

#### **References:**

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 C.I.C Crucho, J. Avó, A.M. Diniz, S.N. Pinto, J. Barbosa, P.O. Smith, M. Berberan-Santos, L.O. Pålsson, F.B. Dias, *Front. Chem.*, 2020, *8*, 404



### Valorization of olive wastes to develop food bioactives using ionizing radiation

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Olive pomace is an environmentally detrimental waste from the olive oil industry that contains a variety of phenolic compounds in considerable contents with potential use as food bioactives. Ionizing radiation has been described as a clean and promising technology to enhance the extractability of bioactive compounds. Thus, this work was carried out with the aim of using ionizing radiation to improve their extractability of the phenolic compounds present in olive pomace as well as to evaluate the possible use of the extracts obtained under optimized conditions to preserve fresh fruit.

The irradiation experiments were carried out at room temperaure in a Co-60 semi-industrial facility (Campus Tecnológico e Nuclear). Regarding the phenolic profile, hydroxytyrosol was found as the most abundant compound in the extracts of olive pomace, followed by hydroxytyrosol-1- $\beta$ -glucoside, tyrosol, luteolin-7-O-rutinoside, oleuropein aglycone isomer 1, and verbascoside. Gamma radiation at 5 kGy improved the extractability of these compounds by 2-fold, as well as the antioxidant activity of the samples. The extraction of the major phenylethanoids present in the extracts from irradiated olive pomace was optimized by heat-assisted extraction (HAE) and ultrasound-assisted extraction (UAE), Compared the obtained optimal conditions, UAE reduced the extraction time and the solvent consumption (t = 28 min, P = 490 W and S = 7.3% ethanol for UAE; t = 120 min, T = 85 °C and S = 76% ethanol for HAE) when compared to HAE, and also led to higher extraction yields (UAE yield = 30%; HAE yield = 13.7%). Nevertheless, HAE extract presented higher antioxidant, antidiabetic, anti-inflammatory and antibacterial activities and no antifungal potential against *C. albicans*. Furthermore, HAE extract also showed higher cytotoxic effect for breast adenocarcinoma (MCF-7) cell line.

The HAE optimized extracts could be incorporated in apples to delay the oxidation of the slices, in order to compare its performance with the commercial antioxidant ascorbic acid. Two different bags (PLA biodegradable film and commercial oriented polypropylene film) were used in packaging the slices. The extract of olive pomace could better inhibit the growth of mesophilic bacteria, filamentous fungi and coliforms until 9 days of storage at 4 °C and preserved the antioxidant potential of the slices, when compared to ascorbic acid. Concerning the physicochemical parameters, the irradiated extracts could preserve texture and color of the apple slices during 9 days.

The overall results indicated that the irradiation at 5 kGy can improve the extractability of bioactive phenolic compounds from the olive waste with a positive impact on the preservation of fresh fruit. These results can support the interest of food industries in developing new ingredients with bioactive potential from agro-industrial wastes, as natural alternatives to the synthetic preservatives and/or additives, contributing for the sustainability of both agro-industrial sector and environment

**Keywords:** olive pomace, ionizing radiation, bioactive compounds, waste valorization, incorporation in food.

#### Acknowledgments

The authors are grateful to the Foundation for Science and Technology (FCT, Portugal): UIDB/04349/2020, UIDB/00690/2020, UIDP/00690/2020, SFRH/BD/136506/2018; the European Regional Development Fund (ERDF): "BIOMA" (POCI-01-0247-FEDER-046112) and "OliveBIOextract" (NORTE-01-0247-FEDER-049865); the "UCASUL - União de Cooperativas Agrícolas do Sul" agro industrial cooperative; the Technological Unit of Radiosterilization (University of Lisbon) for the samples irradiation.

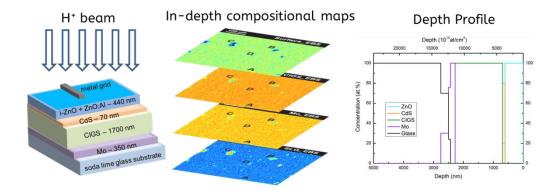


### Nuclear Microprobe: The Tool to Characterize Materials

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The ion beam analytical (IBA) techniques capabilities can be enhanced when coupled to a scanning nuclear microprobe due to the possibility of: i) focusing the beam to sub-micrometer spot sizes and, ii) rastering the area under analysis. In this way, it is possible to obtain elemental distribution maps and the elemental depth profile in a fully quantitative manner. The type of materials characterized in the nuclear microprobe available at CTN-IST is vast and includes, among others: biological tissues and cells, alloys, cultural heritage or semiconductor materials. The analysis can be performed using proton or alpha beams with energy up to ~2.3 MeV which allows to probe the sample at different depths. Examples will be presented to show the versatility of the IBA techniques: i) in-depth inhomogeneities in CIGS solar cell devices (see figure) [1], self-consistent depth profiling and imaging of GaN-based transistors [2]. Also, the use of neural networks to analyze RBS spectra to visualize 3D inhomogeneities will be discussed.



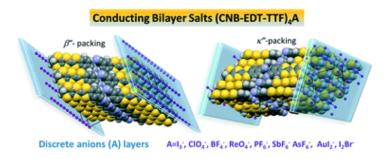
Keywords: Ion beam, characterization, materials, elemental distribution.

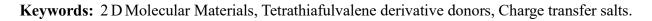


## Conducting bilayer salts (CNB-EDT-TTF)<sub>4</sub>A

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During the last few years a new paradigm of 2D conductors based on molecular bilayers, rather than on single layers, has emerged as a consequence of a series of charge transfer salts based on the organic donor CNB-EDT-TTF (5-cyanobenzene-ethylenedithio-tetrathiafulvalene)[1], with different small anions A (I<sub>3</sub><sup>-</sup>, ClO<sub>4</sub><sup>-</sup>, BF<sub>4</sub><sup>-</sup>, ReO<sub>4</sub><sup>-</sup>, PF<sub>6</sub><sup>-</sup> and SbF<sub>6</sub><sup>-</sup>, AsF<sub>6</sub><sup>-</sup>, AuI<sub>2</sub><sup>-</sup>, I<sub>2</sub>Br<sup>-</sup>, etc...), with general formula (CNB-EDT-TTF)<sub>4</sub>A which has been reported by our group.[2-8] A common structural feature of this series of compounds is the head-to-head arrangement of the donors, induced by a network of weak C≡N<sup>...</sup>H–C interactions, which can be described as an effective combination of R<sup>2</sup><sub>2</sub>(10) and R<sup>2</sup><sub>4</sub>(10) synthons, forming donor bilayers alternating with anionic layers. This series of layered compounds is characterized by a so far unique arrangement of partially oxidized donors in bilayers with interesting two-dimensional metallic or even superconducting properties. They present a rich diversity of polymorphs with different origins: i) different layer packing patterns of donors; ii) alternating or uniform arrangement of donors tilting between successive bilayers; iii) distinct anionic lattices and possible anion ordering schemes. The contribution of the different possible anion layer and interlayer ordering schemes to the structural variations observed will be presented.





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## Novel Radioconjugates for Auger Electron Therapy of Prostate Cancer

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Auger electron (AE) emitters hold great promise for targeted radionuclide therapy (TRT) of cancer, due to their high linear energy transfer (LET) over a nanometric range. When Auger emitters are internalized into highly radiosensitive organelles, such as the cell nucleus or the mitochondria, it is expected that the desired therapeutic effect is achieved with lower administered doses, thus minimizing the side effects. Nuclear DNA has been considered the most relevant target of Auger electrons to have augmented radiotoxic effects and significant cell death. However, the mitochondria are recognized as one of the most important cellular targets to trigger apoptotic reactions and recently are also being studied as a subcellular target for therapeutic AE-emitting radionuclides.

In this context, we have designed dual-targeted <sup>111</sup>In-DOTA complexes carrying a Prostate Specific Membrane Antigen (PSMA) inhibitor (PSMA<sub>617</sub> derivative) and a triphenyl phosphonium (TPP) group to promote a selective uptake by prostate cancer (PCa) cells and their accumulation in the mitochondria, respectively. Conjugates bearing a cathepsin B cleavable linker between the PSMA<sub>617</sub> moiety and the DOTA chelator were also synthesized, aiming at a further enhanced accumulation in the mitochondria upon enzymatic cleavage of the linker (Figure 1). In this way, we expected to obtain AE emitting radioconjugates suitable for a more selective TRT of metastatic castration-resistant prostate cancer (mCRPC).

In this communication, we will report on the synthesis and characterization of novel DOTA-based bifunctional chelators functionalized with PSMA<sub>617</sub> and TPP derivatives and on their respective indium complexes, obtained with <sup>nat</sup>In and <sup>111</sup>In. The preliminary biological evaluation of the radioactive <sup>111</sup>In-complexes was also performed to have a first insight on their potential usefulness for AE therapy of PCa, and will be also presented, including cellular uptake and internalization and PSMA-blocking studies in different cell lines (LNCaP, PC3 PIP and PC3 FLU), and the assessment of radiobiological effects based on the clonogenic survival assay. MicroSPECT imaging studies in PSMA-positive PCa xenografts are underway to assess how the different components influence the *in vivo* behaviour of the radioconjugates.

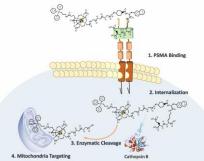


Figure 1. Schematic representation of the proposed strategy for PCa cell targeting of mitochondria.

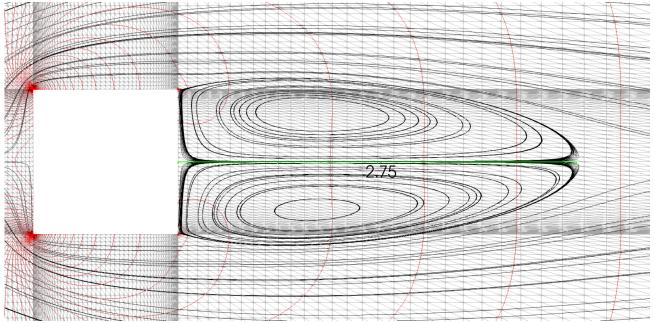
**Acknowledgements:** This work was supported by Fundação para a Ciência e Tecnologia, Portugal (projects UID/Multi/04349/2019, PTDC/MED-QUI/1554/2020). We thank Prof. Martin Pomper, from the Johns Hopkins Medical School (Baltimore, USA) for the kind gift of the PC3 PIP and PC3 FLU cell lines. **Keywords:** Radiopharmaceuticals, Radionuclide Therapy, Prostate Cancer, Prostate Specific Membrane Antigen, Mitochondria



## Hyperisingular Boundary Element Methods (BEM) in Navier-Stokes equations.

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BEM is a well-known numerical method for solving partial differential equations (PDEs). The method was considered for a long time best suited to linear differential equations for which a fundamental solution is available. When an unknown source terms appears in the governing equations, the fundamental function cannot transform the entire problem to one with boundary unknowns only. Thus, discretization of the domain is necessary. In this case the degrees of freedom (dof) can be augmented dramatically which will fill a dense matrix Ax=b for the solution of a system of equations. However, the aforementioned inefficiency of the method can be transformed in to a great gift if numerical techniques are applied. In this presentation they will be addressed techniques applied to BEM methods that remedy this inefficiency. These methods can be the Fast Multipole method (FMM) which was presented by the author in recent works, the meshless Local Boundary Element method (LBIE) and the recently developed Local Domain BEM (LD-BEM). These methods are applied successfully to the non-linear Navier-Stokes equations. The dofs reached by the LD-BEM are more than 10 million in a desktop computer, matching the efficiency of the well-known Finite Element methods. Apart from that, the BEM offers an additional equation, the hypersingular one, which is of great importance in numerous applications. In this presentation, we will focus on the application of the modified BEM methods in the Navier-Stokes and consequently in the importance of the hypersingular equations. It is found very recently that the BEM/FMM is a powerful method capable of solving the Navier-Stokes using exclusively constant elements. In a recent work of the author (to appear in Journal of Computational Physics), the constant triangle is applied to Navier-Stokes obtaining accurate results for pressure and wall shear stress. Comparison with Finite Elements have demonstrated that BEM/FMM can be accurate, robust and a reliable numerical method that merits to be used by modern scientists. In the following figure we can see a resolved flow past a rectangular obstacle using exclusively constant elements.



**Keywords:** Boundary Element Method, Fast Multipole method, Hypersingular equations, wall shear stress, Navier-Stokes, constant elements.



## New Fireproof Dwellings for Wildfire

M.R.T. Arruda\*, P. Cantor, R. Bicelli, J. Firmo e F. Branco \*CERIS-IST-ID, Avenida Rovisco Pais, 1 mario.rui.arruda@tecnico.ulisboa.pt

Although rocket science, computer electronics and biology have evolved to an outstanding level, the science in the protection of home buildings against wildland fires is inexistent, even though the technology to promote its defence is available. This is even more unbelievable, since the cost of the research is very low and known knowledge in fire resistance is much more simple than rocket science or electronics. Therefore, taking into to account the possibility to save thousands of lives every year, the cost-benefit analysis regarding the protection of houses for wildfires is positive.

The main focus of this research project is to protect new dwellings from wildfires, using the concept of a fireproof envelope facade, with existent commercial non-combustible materials.

In 2017, two of the largest wildland fires (WLF) recorded in the history of Portugal (Pedrógão Grande and 15 de Outubro), had a major impact not only on the forest areas (burning 45.000ha+241.000ha respectively), but also on the communities, with a death toll of 114. Following these fires, new legislation was created, only concerning measures related to the wildland-urban interface (WUI) (forest cleaning, vegetation height, distance from vegetation to dwellings, etc...). But interestingly, no extra measure or care was taken, regarding the characteristics of the dwellings or the protection of the people caught by the fires. However, the analysis of expert opinions and questioners, clearly showed that the dwellings that had burned, had constructive typologies without any passive anti-fire protection. The disregard of this aspect, led to the burned houses being rebuilt in the same way as the original, which means that they are likely to burn again in the next WLF.

This important blank in protection measures of new dwellings against WLF, led to the development of this project that aims to fill this gap in knowledge. To solve this problem, fireproof construction guidelines (FCG) with incombustible materials are assembled and tested, for windows, doors, roofs and exterior walls.



Masonry Dwellings





Concrete Dwellings



Wood Roof StructureMasonry Dwellings with Wood RoofExample houses that burned, adapted from Portuguese press SIC, RTP and DN.

**Keywords:** Passive Fire Protection, Wildland Fire, Non-Combustible Construction Materials, New Fireproof Construction Guidelines.



# The role of volcanism as a source of trace elements to the environment: The case of Deception Island - Antarctica

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Deception Island (DI) located in the South Shetland Islands Archipelago near the Antarctic Peninsula is among the most active volcanoes of this region, having erupted at least 6 times since it was first visited around 160 years ago. DI consists of a composite volcano, whose central part is occupied by an 8.5 by 10 km elongated collapsed caldera. Port Foster Bay, the sea-flooded part of the caldera depression, is slightly smaller due to the numerous post-caldera eruptions that occurred around the caldera wall margins.

Some studies in DI showed that the active volcanism is an active source of trace metal contaminants namely Arsenic (As), Copper (Cu), Cadmium (Cd), Lead (Pb) and mercury (Hg) however, the biogeochemical cycle of these elements in this remote system have only been recently studied.

Sources and speciation of the above trace elements were investigated, and a hydrological transport model were developed to trace those elements inside the caldera and their impact to the surrounding Southern Ocean. Organisms' accumulation was also studied.

Results showed that in saline waters, Cu and Pb had important punctual sources, and that concentrations of Cd and Hg were consistently high pointing to the existence of a natural and diffuse source related with the hydrothermal activity. Environmental conditions inside the caldera were found to be optimal for Hg methylation (formation of the toxic methylmercury) with measured rates higher than in other polar systems. These results coupled with a higher resident time of water inside the caldera suggest a potential impact in the living organisms due to the accumulation of the studied trace elements in caldera waters.

This work clear indicates the impact of active volcanism as a source of natural contamination and their potential role on the local, regional and global biogeochemical cycles, which is far for being taking into account in the current models..

Keywords: Volcanism, Trace Elements, biuogeochemical Cycle, Deception Island, Antartica



## **Conceptualizing Socio-Tech Entrepreneurship**

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#### Why does this research matter?

- Inequality is growing both in developing and developed countries, which exacerbates divisions and slows economic and social development
- Technology plays a significant role in scaling social impact, contributing to accelerating the achievement of the 2030 SDG
- Socio-Tech Entrepreneurship is a growing observable phenomenon, often referred to as «tech4good»
- There is almost no scientifically peer-reviewed conceptual research on Socio-Tech ventures.

#### What was the research process?

Through a Systematic Literature Review of Technology Entrepreneurship (TE) and Social Entrepreneurship (SE), it was possible to:

1) Understand what Socio-Tech Entrepreneurship has in common with and how it differs from TE and SE

- 2) Propose a conceptual framework for Socio-Tech Entrepreneurship (STE)
- 3) Open future research avenues.

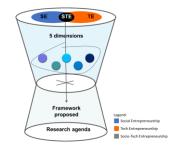


Figure 1 - Methodological process followed

#### What is the contribution of this research?

This research develops a comprehensive assessment of Socio-Tech Entrepreneurship to propose a conceptual framework summarizing state-of-the-art knowledge and opening future research avenues.

#### Will this research make a difference?

Yes. By serving as a solid ground for future usage of technology by all stakeholders involved.



Figure 2 - Expected contributions of this research

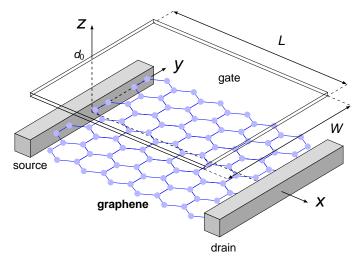
**Keywords:** Technology-based Entrepreneurship, Social Entrepreneurship, Socio-Tech Entrepreneurship, Systematic Literature Review, Research Agenda



### Plasmonic Instabilities in two-dimensional Dirac Materials

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The generation of coherent terahertz radiation is an outstanding challenge at both scientific and technological levels. In one hand, the quest for table-top THz solutions based on integrated-circuit technology puts graphene and other bi-dimensional in the run. Plasma instabilities in bi-dimensional materials are an appealing mechanism for the production of low-power coherent THz signals. In this talk, we discuss how to produce plasmonic instabilities based on electronic injection only in field-effect transistors made of graphene (see Fig. 1).



**Figure 1:** Schematic representation of a graphene field-effect transistor. A dc source-to-drain current is applied, while the gate locally controls de Fermi level of the conductors. By acting with additional tension and current sources at the source and drain, asymmetric boundary conditions allow for a dc to ac conversion of the plasma signal, leading to the emission of coherent THz radiation.

Keywords: Graphene, Dirac Materials, Plasma Instabilities, THz radiation.



### Ion beam analysis of Li-Sn alloys

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Alternative concepts of plasma facing components (PFCs) are based on the use of liquid metals (LM) wetting W PFCs [1]. The reactivity of Li, Sn and Li-Sn alloys with W is low [1,2]. Liquid Sn can be used in a wide temperature range in operative scenarios [2]. The shortcomings of liquid Li are the lower operative temperatures (up to ~500 °C), a high affinity to react with H and O [2] and the high melting points of Lirich intermetallics [3]. Nevertheless, the transport of Li to the plasma edge reduces turbulence and increases confinement [2] and therefore, Li-Sn alloys with low Li contents may be a good alternative for LM applications. They are being produced at IST with target compositions up to 25 at.% Li via mechanical alloying (MA) by milling pure Sn powders and Li ribbons under dry Ar. Distinct MA parameters were followed to assure an effective reactive milling and improved Li-Sn alloying.

Ion beam analysis is suitable to help optimizing the MA procedure by characterizing the elemental composition of the pristine materials and of the modifications imposed by MA, air exposure and plasma irradiation.

Apart O contents less than 1 at.% attributed to both Sn and Li sources, proton induced X-ray emission

(PIXE) pointed Pb ( $\leq 0.05$  at.%), a natural contaminant of Sn, and Fe ( $\Box 0.05$  at.%) abraded from the stainless steel vial and milling balls, as the sole contaminants of the alloys. Elastic backscattering spectrometry (EBS) allows depth profiling of O by following the <sup>16</sup>O(p,p)<sup>16</sup>O reaction yield and the decrease of the Sn backscattering yield in the surface layers due to the migration of Li to react with O. Simultaneously, accurate depth profiling of Li down to depths of 10-20  $\Box$ m is achieved by nuclear reaction analysis (NRA) with the <sup>7</sup>Li(p,<sup>4</sup>He)<sup>4</sup>He reaction, evidencing losses of Li lower than 10 % during the MA stage. Elemental mapping with a nuclear microprobe indicates that Li spreads across the Sn grain powders. Despite the competitive <sup>2</sup>H(<sup>3</sup>He,p)<sup>4</sup>He, <sup>6</sup>Li(<sup>3</sup>He,p)<sup>8</sup>Be, <sup>7</sup>Li(<sup>3</sup>He,d)<sup>8</sup>Be and <sup>7</sup>Li(<sup>3</sup>He,p)<sup>9</sup>Be nuclear reactions, the retention of <sup>2</sup>H in irradiate samples is quantified by using <sup>3</sup>He<sup>+</sup> ion beams of 1 MeV energy.

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[2] R.E. Nygren, F.L. Tabarés, Nucl. Mater. Energy 9 (2016) 6.

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Keywords: Ion beam analysis, XRD, electron microscopy, lithium-tin alloys, nuclear fusion



## **Optimization of Alpha Particle Confinement in Fusion Devices**

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The design of reactor relevant fusion devices with full three-dimensional topological properties, also called stellarators, has been historically performed using target objective functions computed using codes that computed magnetic field equilibria that satisfy the ideal magnetohydrodynamic equations. Such approach suffers from inherent shortcomings, such as the dependence on initial conditions and the numerical method employed. Furthermore, due to the numerical cost involved, such approach is not suited for surveying the entire space of magnetic configurations and offers relatively little insight into the space of solutions. In this work, we use a new paradigm for rapid stellarator configuration design with a lower number of free parameters in the optimization procedure. This is made possible by computing the flux surface shapes directly using an expansion in large aspect ratio. This approach is valid for the inner region of any stellarator device. Using this approach, we can advance the understanding of energetic particle confinement in stellarator devices, which has long been thought of as a weak point in nonaxisymmetric configurations. Although quasisymmetric and omnigenous stellarators can reduce neoclassical losses to acceptable levels, energetic losses, such as those from alpha particles in stellarator fusion reactors, can be higher than the allowed engineering limits of the device and are enhanced by unavoidable deviations from the idealized equilibrium magnetic field. Using a particle tracer code able to evolve both the full orbit and the guiding-center orbits of energetic particles, we characterize the losses of energetic particles in non-axisymmetric equilibria and optimize the equilibrium solutions to minimize such losses (see example in Figure 1). By combining a numerically efficient algorithm with analytical methods, we find a set of configurations applicable to the core of any stellarator device with good fast particle confinement. In addition to providing key physical insight, these configurations can be used as initial conditions to standard optimization methods to improve their efficiency and reliability.

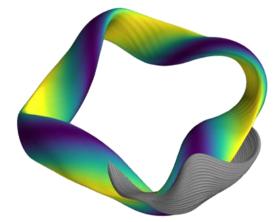


Figure 1: Trajectory of an alpha particle in an optimized quasi-helical stellarator (grey). The toroidal surface corresponds to the magnetic field equilibrium and the colours represent the modulus of the magnetic field strength.

Keywords: Nuclear Fusion, Plasma Physics, Stellarator Optimization, Numerical Methods, Magnetic Confinement



## Influence of culture media on Mesenchymal Stromal Cell expansion and hematopoietic support capacity

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Over the last few years, *ex-vivo* expanded Mesenchymal Stromal Cells (MSC) have been intensively studied due to their therapeutic potential for several conditions. Nevertheless, clinical trials are often withdrawn due to contradictory results. Different sources, isolation methods, or culture conditions can originate MSC populations with different properties leading to conflicting results. In this work, the influence of culture media (serum-containing *vs* serum-free supplemented culture media) on human bone marrow-derived MSC expansion and functionality were studied.

For that, three MSC donors were cultured for 4 passages with basal culture medium (DMEM) supplemented with human Platelet Lysate (DMEM/hPL) or Fetal Bovine Serum (DMEM/FBS), in three scenarios: (1) continuously in the same medium, (2) adapted to a different medium halfway, and (3) adapted to a different medium and then re-adapted to the original one. At each passage, the number of MSC obtained, their morphology, and the expression of CD146 and CD271 were assessed (surface markers thought to be associated with MSC hematopoietic support capacity). After the last passage, MSC from the three scenarios aforementioned were co-cultured with Hematopoietic Stem/Progenitor Cells (HSPC) to evaluate their hematopoietic support capacity.

It was found that culture media affected MSC's properties: when grown in DMEM/hPL, MSC were smaller and had a higher growth rate and a higher expression of CD271 surface marker. Regarding the CD146 surface marker no conclusion could be made across the three donors. Moreover, MSC expanded with DMEM/FBS in the last passage, regardless the culture medium used in the previous passages, originated a higher number of TNC and a higher percentage of CD34<sup>+</sup> cells after 7-day expansion of HSPC. Overall, it can be concluded that culture media affect MSC's phenotype and function and therefore it is one of the factors that should be considered when developing MSC-based therapies.

**Keywords:** Mesenchymal Stromal Cells; Hematopoietic Support; Human Platelet Lysate (hPL); Fetal Bovine Serum (FBS).



## Manufacturing cultured meat through a scalable and cost-effective bioprocess

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In recent years, there has been an increasing interest in cellular agriculture, an emerging field that aims to overcome most issues associated with livestock meat consumption, such as its environmental impact, risk of foodborne diseases and animal slaughtering. Different approaches have been attempted to produce cultured meat, but high production costs and scalability limitations have hampered this technology. Bioprocess scale-up is crucial to ensure the product's economic viability and availability, so key factors must be optimized, such as the cell source, bioreactor systems, culture medium, scaffolding and biomaterials to support cell proliferation and achieve the desired properties. To address this, our work focused on optimizing cell proliferation and differentiation into relevant cell lines under static conditions. Mesenchymal stromal cells (MSC) were chosen as the starting cell line for their high proliferation potential and ability to differentiate into myocytes (the principal constituent of meat) and adipocytes (which contribute to the organoleptic properties of meat). MSC isolation from bovine umbilical cord was successfully performed, and the cells were characterized and expanded under different 2D culture conditions. Future studies will focus on optimizing cell proliferation and differentiation, both under static and dynamic conditions. It is foreseen that this work will build the foundations for an innovative platform to produce cultured meat with good consumer acceptance in a cost-effectively and at a large-scale manner, increasing the availability of alternatives to livestock meat.

**Keywords:** Cellular agriculture; Cultivated meat; Bovine Mesenchymal Stromal Cells; Myocytes/Adipocytes; Scalability



# Purification of small heat shock protein nanocages: exploring a chromatographic approach

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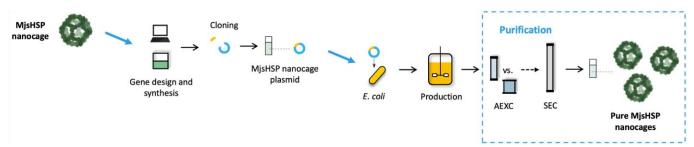
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Protein nanocages are versatile vehicles for biomedical applications. These nanometer scale architectures feature an inner cavity that can be loaded with different molecules. The clinical development of protein nanocages requires large amounts of pure, well-folded assemblies. However, while the currently used purification approaches are suitable for proof-of-concept studies at lab scale, biomanufacturing at large scale will require more efficient bioprocess technologies to enable the use of protein nanocages in clinical applications. The main objective of this work was to develop scalable and cost-effective processes for the biomanufacturing of protein nanocages with particular emphasis in the downstream processing steps. The 16.5 kDa small heat shock protein from Methanococcus jannaschii (MjsHSP) was used as model. The in vivo assembly of 24 units of MjsHSP originates 12 nm nanocages with octahedral symmetry and demarcated exterior and interior surfaces. The nanocages were produced in E. coli and in an alternative expressing host (Vibrio natriegens). The purification strategy consisted of an intermediate purification followed by a polishing step to achieve a highly purified and formulated product. Different approaches of chromatography (anion exchange, size exclusion and multimodal) as well as traditional and novel chromatographic supports with distinct properties were tested and analysed. The pure MjsHSP nanocages were analysed by SDS-PAGE and characterized by dynamic light scattering, fluorescence correlation spectroscopy and transmission electron microscopy. The obtained results demonstrated that a downstream processing strategy based on two chromatography steps could be an efficient platform to obtain pure protein nanocages for pre-clinical/clinical applications.

<u>Acknowledgments</u>: The authors acknowledge the funding received for the iBB-Institute for Bioengineering and Biosciences from FCT-Fundação para a Ciência e a Tecnologia (Project UIDB/04565/2020 and UIDP/04565/2020) and from Programa Operacional Regional de Lisboa 2020 (Project N. 007317) and for the i4HB-Associate Laboratory Institute for Health and Bioeconomy (Project LA/P/0140/2020). Funding from FCT through the PhD fellowships to Jorge João (PD/BD/150335/2019, BIOTECnico PhD Program) and to Sara Sousa Rosa (SFRH/BD/148437/2019) is also acknowledged.

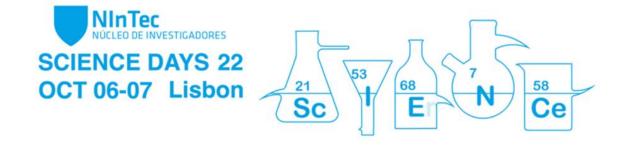
#### **Figure/Scheme:**



**Keywords:** protein nanocages; small heat shock proteins; biomanufacturing; downstream bioprocessing; chromatography



NInTec Science Days (6-7 October 2022)



## October, 6 Poster Session



## Sustainable Blood Supply Chain Network Optimization: Location-Allocation Approach adding Transshipment Strategy

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A location-allocation problem involving healthcare facilities with blood services and related institutions is studied. An integrated multi-objective and mixed-integer linear programming model is proposed aiming to achieve strategic and tactical planning of the Blood Supply Chain (BSC) network. Firstly, and under a deterministic demand, geographical distribution for donors/patients is considered, allowing the definition of supply/demand allocation of facilities, as well as product flow calculations with transshipment applied among demand facilities. Next, the model is extended to consider demand as an uncertain parameter. The objective functions consider a sustainable mindset, namely by addressing the minimization of transportation costs and blood product loss costs. The application of the proposed model is demonstrated with a Portuguese case study with the respective scenarios. The results are analyzed, discussed and some conclusions are drawn.

Keywords: Facilities Planning and Design, Optimization Modeling, Sustainability, Transshipment



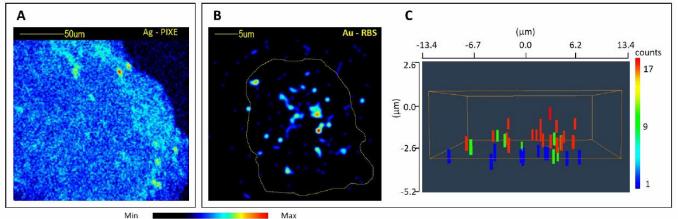
Energetic ion beams for nanotoxicology and therapeutic applications

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Over recent years we have experienced an increase in the use of nanoparticles and other metal-based complexes for a variety of applications, such as, in technology, food and cosmetics industries, and (bio)medical areas. A considerable amount of research have evolved focused on these chemical entities for different cancer therapeutic modalities. The increased use of these chemical entities raised several concerns on their potential toxicity. In (bio)medical areas, it is urgent to explore how these entities interact with biological systems. One approach can be to quantitate the net amount uptake by cells and tissues. Other approach encompasses the direct visualization of the distribution of the metal content in the cell volume. This is essential to evaluate the uptake of the complexes and nanoparticles and anticipate their biological effects. Due to their small size, the identification and localization within cells is extremely challenging. Various cutting-edge techniques are required to detect and quantify metals and electron-dense nanoparticles inside the cells. However, few of these techniques are able to peer into cells combining nanometer probeformation with elemental quantification and depth profile of the element of interest production 3D maps of its distribution inside cells. This is the prospect of nuclear microscopy techniques using MeV ion beams.



**Figure 1**. Nuclear microscopy delivers elemental distribution and depth profile images with high-resolution. A – distribution of silver nanoparticles at the surface of wastewater granules (microbial populations); B – distribution of a gold complex in a PC3 cell (human prostate cancer cell); and C – the gold depth profile in the same cell. The cellular uptake can be visualized and its preferential localization identified.

Keywords: Nuclear microscopy; metals, nanosized complexes, nanoparticles, cellular uptake



# Synthesis and irradiation response of high entropy alloys with transition and refractory metals for nuclear fusion

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due to their innovative properties. However, their unconventional compositions and chemical structures hold promise for achieving unprecedented combinations of mechanical properties, microstructures and irradiation resistance for the use in extreme environments. In this work results on two types of HEAs will be presented: based on transition metals (CuCrFeTiV) and refractory metals (CrNbTaVW). All the alloys were prepared by ball milling followed by consolidation by spark plasma sintering and then irradiated with Ar ions in order to check the adequacy for use as a thermal barrier in future nuclear fusion reactors. Structural changes were investigated by X-ray diffraction, and scanning electron microscopy and scanning transmission electron microscopy, both coupled with X-ray energy dispersive spectroscopy. Surface irradiation damage on CuCrFeTiV was detected for high fluences ( $3 \times 10^{18} \text{ Ar}^+/\text{cm}^2$ ) with formation of blisters of up to 1 µm in diameter. Cross-sectional scanning transmission electron microscopy showed the presence of intergranular cavities only in the sample irradiated with  $3 \times 10^{18} \text{ Ar}^+/\text{cm}^2$ , while all irradiation experiments produced intragranular nanometric-sized bubbles with increased density for higher Ar<sup>+</sup> fluence. Moreover, no severe superficial modifications were observed in the CrNbTaVW samples, after irradiation at different temperatures.



### Activation of CO<sub>2</sub> and other unsaturated molecules by uranium bis(aryloxide) cyclam complexes

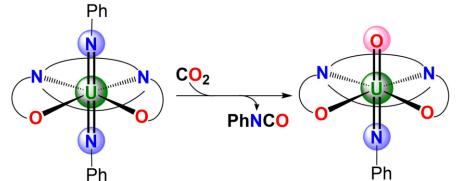
L. Maria,<sup>1,\*</sup> N. A. G. Bandeira,<sup>2</sup> J. Marçalo,<sup>1</sup> I. C. Santos,<sup>3</sup> J. K. Gibson<sup>4</sup>

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Uranium chemistry has a unique history closely connected to applications in nuclear energy that have determined the evolution of its research. The initial focus was on preparation of volatile compounds for uranium isotopic separation, a needed step in the fabrication of nuclear fuel. Later, and continuing to the present, studies concentrated on separation of spent fuel and elimination of waste from nuclear power plants and weapons dismantling, and related environmental issues. Notably, as nuclear energy is currently a candidate for carbon-neutral energy, there is an enticing prospect to utilize the depleted uranium by-product of isotope enrichment. These topics promoted the development of uranium chemistry but neglected important subtopics with a consequence that uranium chemistry has historically lagged behind that of most d-transition metals.

In the last two decades, there has been a resurgence of uranium coordination chemistry, particularly in the non-aqueous realm [1]. In most studies directly relevant to nuclear applications, aqueous systems are preponderant and uranium chemistry is dominated by the particularly stable hexavalent uranyl moiety, *trans*- $\{O=U=O\}^{2^+}$ . In anhydrous organic solvents and using special synthetic procedures, novel complexes with diverse uranium-ligand bonds and oxidation states (+2, +3, +4, +5, +6) can be prepared to address more varied aspects of fundamental uranium chemistry, such as the nature of bonding and its effect on reactivity and properties. Although uranium is only mildly radioactive, this is a hindrance to industrial applications unless sufficiently unique and useful chemical transformations are identified.

We use synthetic chemistry, structural characterization, specialized spectroscopic studies and quantum chemistry computations in a synergistic effort to understand uranium-ligand bonding and reactivity. In our recent work [2-4], we utilized uranium complexes supported by a bis(aryloxide) cyclam ligand to activate unsaturated molecules, namely azobenzenes, carbon dioxide and nitrite, and to form uranyl analogue species, *trans*-{E=U=E}<sup>2+</sup> (E = O, NR) [5].



Activation of  $CO_2$  by a U(VI) bis(imido) complex with release of phenyl isocyanate.

**Keywords:** uranium, bis(aryloxide) cyclam, carbon dioxide activation, uranium-ligand multiple bonding, uranyl analogues.

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### Carbon dioxide capture and utilization for energy storage

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The European Green Deal has the overarching aim of making Europe climate neutral in 2050, but the global energy consumption is expected to continue growing. Post-combustion  $CO_2$  capture based on regenerable sorbent materials at high temperatures has received increasing attention as an alternative to low-temperature  $CO_2$  capture and conventional chemical absorption systems. Ca-Looping (CaL) is one of the most promising technologies for post-combustion  $CO_2$  capture (Fig.1) based on the reversible chemical reaction

of CaO and CO<sub>2</sub> to form CaCO<sub>3</sub>. The high sorption capacity (0.78 g CO<sub>2</sub>/g CaO), high selectivity, the use of inexpensive sorbents and the synergy with cement production due to the possible utilization of these exhausted sorbents as raw materials for the cement industry, are the main advantages of this CO<sub>2</sub> capture process. The enhancement of CaL process performance has been successfully assessed at CQE/IMS/IST laboratories through the development of nano CaO sorbents by sol-gel method [1], CaO-Al<sub>2</sub>O<sub>3</sub>-based pellets [2], blending of natural sorbents [3] and addition of inert wastes [4].

In addition, CaL application in thermochemical energy storage (TCES) is being focus of research. TCES consists of using the high temperatures attainable in a concentred

solar power (CSP) plant to drive an endothermic chemical reaction, and when energy is needed, the stored reaction products are brought together at the necessary conditions to drive the exothermic reverse reaction. The high energy storage density of CaCO<sub>3</sub> (1790 kJ/kg), and the high temperatures used during carbonation allow attain high power cycles efficiencies (ca. 44-45 % for the CO<sub>2</sub> closed Brayton cycle), which makes CaL process an interesting alternative as demonstrated in our studies [5].

Recently, the CO<sub>2</sub> capture by MgO sorbents at mediumtemperature (200-400 °C), that can be used in both post and pre-combustion CO<sub>2</sub> capture technologies has been also investigated at CQE/IMS/IST laboratories. The MgO sorbents have a high theoretical carrying capacity (1.09 g of CO<sub>2</sub> /g of MgO), affordable price, availability, and a medium regeneration temperature (~500 °C). The highest drawback of MgO is its poor sorption capacity coupled with slow kinetics and low thermal stability. To enhance CO<sub>2</sub> carrying capacity of MgO sorbents it was applied successfully several techniques: synthesis of nanosized MgO, dispersion of MgO on porous inert supports, use of different precursors and alkali doping (Fig. 2).

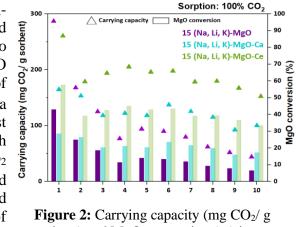
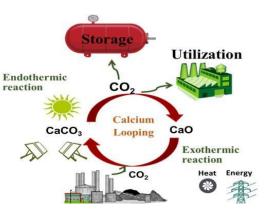


Figure 2: Carrying capacity (mg  $CO_2$ / g sorbent) and MgO conversion (%) in a fixed bed reactor

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8494; [2] Journal of CO<sub>2</sub> Utilization 2022, 102007; [3] Materials 2021, 14(16): 4379; [4] Separation and Purification Technology, 2020, 235: 116190; [5] Journal of CO<sub>2</sub> Utilization, 2022, 65:102180

Keywords: High and medium temperature CO<sub>2</sub> sorbents, Ca-looping, MgO-based sorbents, thermochemical energy storage



**Figure 1:** Calcium looping process for CO<sub>2</sub> capture and thermochemical energy storage



### Magnetic, Luminescent and Thermochemical case study of the [C<sub>2</sub>mim][Ln(fod)<sub>4</sub>] series (Ln = Nd-Tm except Pm)

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A series of nine Ln complexes of the type  $[C_2mim][Ln(fod)_4]$  were prepared and their thermochemical, photophysical and magnetic properties were evaluated. Thermochemical studies presented a rare and reversible conversion between two solid phases, characteristic of the  $[Ln(fod)_4]^-$  anion. The photophysical and magnetic studies revealed that the Dy and Er presented the multifunctionality of being simultaneously SMMs and Visible (Dy) or Near Infra-Red (Er) emitters. The Nd, Ho and Tm analogues present characteristic emission bands in the NIR region (800-1200 nm), while the Sm, Eu, Tb and Dy present emissions in the visible range. Magnetic susceptibility of complexes Tb, Dy, Ho, Er and Tm showed paramagnetic behaviour, although with different regimes, with Gd, Dy and Er presenting SMM behavior.

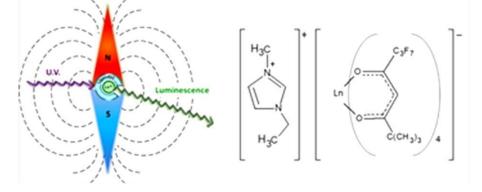


Figure: Multifunctionality within the [C<sub>2</sub>mim][Ln(fod)<sub>4</sub>] series.

Keywords: Lanthanides; Luminescence; Magnetism; Thermochemistry; Polymorphism.

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# High-temperature vapor-liquid equilibrium for the systems water+methanol and ethanol+butanol and modelling with the software ASPEN PLUS V11

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Vapor-liquid equilibrium data gives the behavior of mixtures with the temperature or pressure. This type of information is very important to design the separation units in industry. The cost of separation contributes significantly to the total cost of production, making VLE one of the most important properties in chemical engineering. However, there are two main problems, it is difficult and expensive to obtain accurate experimental data and it is not possible to retrieve data for all the important systems. The other problem is that some data available are not accurate or thermodynamic consistent. These two problems lead to an erroneous process design that can causes losses in the order of millions of dollars to industry.

Alcohols are an extremely essential chemical. They are widely used in industry as solvents for fats, oils, resins, paints, and nitrocellulose; others are used in the production of fragrances and braking fluids. They can also be used as biofuel. The price of crude oil is rising, making biofuel production processes competitive with fossil fuels. [1] Another very important question is the targets that Europe needs to achieve until 2030. By 2030 the target is to reduce 55% of the carbon emissions in Europe.[2] To achieve this biofuels are one of the solutions. The ABE (Acetone, Butanol, Ethanol) process can be used to make biobutanol, the most similar alcohol to gasoline. This process consists of a pre-treatment and fermentation of the biomass, and then a separation of the butanol by distillation. Distillation plays a major role in optimizing this process, making VLE data the key to this process.[2][3]

In this project accurate VLE data at high temperatures will be presented for the mixtures water + methanol and ethanol + butanol. Software ASPEN PLUS V11 will be used for modelling the systems retrieving new NRTL parameters.

Keywords: Vapor-Liquid equilibrium, ethanol, butanol, Aspen Plus, Modelling

Acknowledgements: Support for this work was provided by FCT through UIDB/00100/2020 and UIDP/00100/2020. Institute of Molecular Sciences is an Associate Laboratory funded by FCT through project LA/P/0056/2020. B.P. Nobre acknowledges IST and FCT for the Scientific Employment contract.

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## A new type of biomass as support for pigment degradation

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In this work in a new type of biomass - insect exuviae have been made and used as support for copper acetate(II), to assess the impact of different parameters such as the size of the particles, the temperature, and the degradation of colorants regarding the resistance, the flexibility, and the viability. FTIR analysis and microscopic observations are made to compare the different results and to explain the different behaviors of each sample.

Keywords: biomass, Copper, pigments



## Bio-oil production using ionic liquids as catalysts

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Compared with organic solvents, ionic liquids are considered cleaner solvents due to their certain peculiar properties, such as good thermal stability and unique solvation ability. Therefore, it is intended to create an environment-friendly reaction medium with these liquids.

This work aims to analyse the effect of ionic liquids and organic solvents on the liquefaction of biomass to produce bio-oil, from the conversion of different biomasses, namely, pine wood chips and *acacia saligna*. Results and discussion of the performance of different ionic liquids, as well as molecular organic solvents, will be presented, along with the characterisation of the biomass, solvents, and bio-oils.

Keywords: Bio-oil, ionic liquids, biomass

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# Neutron-gamma and pile-up discrimination aiming at plasma real-time control in nuclear fusion experiments

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Nuclear fusion is a potential candidate for energy production in the coming century. One relevant challenge in its development is both scientific and technically challenging: how to control plasma in destructive environments. Real-time plasma control relies on massive amounts of information from diagnostics tools. One of these diagnostics is the neutron emissivity profile, which requires the processing of hundreds of thousands of pulses each second. Neutron generating processes in fusion are associated with the emission of gamma rays, which makes discrimination of neutrons from gammas in a detector a necessity. In a high count-rate environment, the probability of superimposed pulses, or pile-up, can be a significant proportion of events. Pile-up rejection and statistical compensation can mitigate its statistical effect. Pulse-Shape Discrimination (PSD) algorithms discriminate neutrons from gammas, but accurate algorithms are generally too slow or computationally intensive to apply in plasma control in real-time, in particular for discriminating particle types in piled-up signals.

Monte-Carlo simulation is used to generate custom waveforms, based on a known semi-empirical equation that parametrizes scintillation pulse shapes according to an exponential decay rate and exponential rise time. This well-studied waveform is used in a template-matching pile-up separation algorithm, mixed with a recent PSD offline approach, by rating each pile-up event against all possible neutron-gamma template combinations. It is found that the algorithm can adequately perform PSD in piled-up pulses using real data. With the computationally expensive portion of the algorithm being performed in calibration, it has the potential for real-time usage.

Keywords: PSD, pile-up, ITER



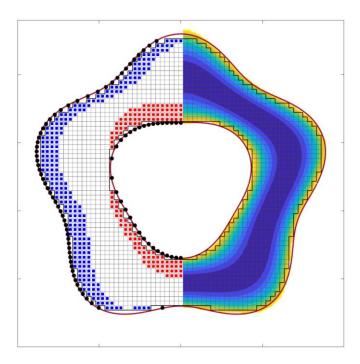
## A Simplex Immersed Boundary Method for Very High-Order Numerical Schemes

B. F. S. Delgado; D. M. S. Albuquerque<sup>\*</sup> \* Corresponding author IDMEC, Instituto Superior Técnico, Universidade de Lisboa, Lisboa, Portugal. duartealbuquerque@tecnico.ulisboa.pt

High-order numerical schemes, while more complex to implement, provide a higher numerical accuracy for the same computational time or cost. The application of Immersed Boundary Methods allows for the simulation of an embedded body without the use body-fit grid, which is suitable for fluid-structure problems.

A very high-order immersed boundary method based on a simplex line approach is proposed. The classical way to solve this is through a polynomial reconstruction of the immersed boundary, using 2D stencil and the least-squares method. This new method consists in a 1D stencil for each solid point and solving the extended global matrix from the problem. Two approaches that impose values near the solid region are tested: an interpolation using the boundary value and surrounding information of the grid; and a central flux reconstruction by considering additional extrapolated ghost points inside the solid domain.

These approaches are tested and compared in the 1D space, with the polynomial interpolation (first and novel approach) showing better results. Both Dirichlet and Neumann boundary conditions were verified, polynomial reconstruction of equal to the order (O) and plus one the order (O+1). In the 2D space, the interpolation method is submitted to further investigation. The error convergence rates are compared against other numerical results from the literature, including the classical Taylor-Couette problem and other more complex geometries (see rose-shape example from the figure).



**Keywords:** Immersed Boundary Method; High-order Scheme; Finite Volume Method; Least Squares Method; Convection-Diffusion Equation.

#### Acknowledgment:

Both authors acknowledge the financial support received by FCT under the research project: High-order immersed boundary for moving body problems HIBforMBP. **Reference**: PTDC/EME-EME/32315/2017.



### Ion Beam Analysis (IBA) of materials - from old to new

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Adding versatility to accuracy and sensitivity, IBA techniques have been applied to a wide number of scientific fields, including Material Science, Biology/biomedicine and Cultural Heritage (CH). Coupled to a Nuclear Microprobe, all the capabilities of IBA are extended in order to give sample information with lateral spatial resolution while adding imaging possibilities. Here we show some case studies carried out at the Laboratory of Accelerators and Radiation Technologies from IST in collaboration with external or internal researchers with work focused on the characterization of functional materials and CH artefacts.

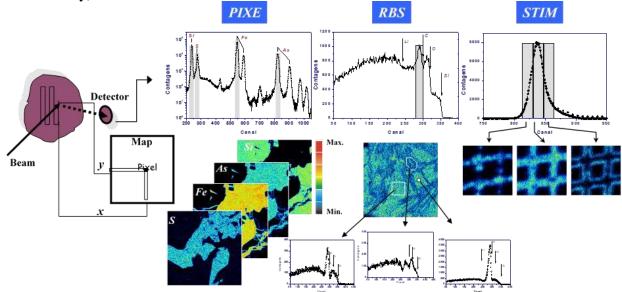
#### CH:

#### Glass, stained glass and enamels;

In the CH field several types of artefacts have been characterized from historical glasses (aiming to determine the raw materials used, their production techniques and provenance) to ancient gold artefacts (aiming to determine base alloys composition and identify manufacture techniques those may involving joining techniques with the determination of solder alloys composition) and other CH materials such as paintings (paint pigments identification of the artist colour pallet used that may contributing to their authenticity evaluation or identification of modern intervention areas).

#### **Functional Materials:**

With  $\mu$ m lateral spatial resolution and possibility of obtaining in-depth profile information on elemental distribution, the results that can be obtained are important to define needed improvements on the devices manufactures. Studies carried out involved several different types of devices, from perovskites and CIGS solar cells (surface film coverage, elemental composition and their depth profile are very important for attaining a high efficiency solar cell with a proper band-gap) to under development radiation sensor devices such as Ga<sub>2</sub>O<sub>3</sub> micro-flakes or GaN microwires (perform electrical measurements during and after irradiation with MeV ion beams) and also considering the cytotoxicity evaluation of developed polymers for biomedical applications (PE-g-HEMA films prepared by gamma irradiation at the IST 60Co source irradiation facility).



Keywords: Nuclear microprobe, historical glass and artefacts, solar cells, radiation sensors, PE-g-HEMA



# Microfluidics for development of alginate microparticles co-encapsulating cells and growth factors

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Hydrogels are very useful in wound healing, since they can retain large amounts of water, keeping a moist environment for wounds and assisting tissue recovery. Mesenchymal stem cells, as well as growth factors, such as insulin, are ideal candidates for wound healing applications that can be loaded into microparticles and incorporated in a hydrogel for different applications [1]. Within different techniques available for cell microencapsulation [2], microfluidics was chosen due to its versatility of designs and the real-time control of processing parameters, such as microparticle size, frequency of loaded cells and co-encapsulation with drugs. Therefore, the aim of this work was to develop a microfluidics device for delivery of alginate microparticles to be used for co-encapsulation of mesenchymal stem cells and insulin, as a growth factor model. Thus, alginate microparticles have been successfully obtained with a spherical shape and smooth surface using a PMMA (poly(methyl methacrylate) device with a T-junction conformation and two immiscible liquids, specifically alginate solution of 1.2 % (m/v) and lipidic maisine CC. However, the used PMMA device needs further optimization, which would include a microparticle precipitation and washing phase. This system should allow the development of a continuous microparticle co-encapsulation of cells and growth factors and, at the same time, protect cells from stress and maintain cell viability and functions for an effective drug delivery.

Keywords: Mesenchymal stem cells; Microdroplet; Microparticle; Hydrogel; Wound healing

Acknowledgments: This work was funded by Fundação para a Ciência e a Tecnologia (FCT) in the scope of the projects UIDB/04326/2020, UIDP/04326/2020 and LA/P/0101/2020 of the Research Unit Center for Marine Sciences—CCMAR, and UIDB/04565/2020 and UIDP/04565/2020 of the Research Unit Institute for Bioengineering and Biosciences—iBB, and LA/P/0140/2020 of the Associate Laboratory Institute for Health and Bioeconomy—4HB.

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# Polyelectrolyte Capsules as Smart Toolboxes towards Light Triggered Processes

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In recent years, polyelectrolyte microcapsules (PECs) have received a great deal of attention due to their possible use as drug delivery systems, biosensors, and micro-reactors. The integration of light-absorbing molecules such as porphyrins, within these platforms enables the production of optically addressable devices [1-3]. Porphyrins are recognized photosensitizers for cancer treatment and diagnosis, due to their intrinsic ability to generate cytotoxic oxygen species and to emit in the red or near infrared when exposed to visible light. Nevertheless, most porphyrins are weak emitters, have solubility issues, and tend to aggregate in water.

Herein we report some of the 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 [2]. Further, PECs were also employed as micro-reactors for the construction of needle like porphyrin J aggregates [3]. Recently, we have shown that PECs are valuable platforms towards the preparation of spectrally engineered microsystems for efficient plasmonic fluorescence enhancement of porphyrins [4]. Fluorescence lifetime imaging microscopy of porphyrin-nanogold PEC hybrid data reports a notable  $10^5-10^6$ -fold increase in the maximum detected photon rates from diffraction-limited spots and an overall six-fold increase in fluorescence as averaged over the whole microcapsule area. The cytotoxic activity of porphyrin-nanogold PECs hybrid in HeLa Cells originating from human adenocarcinoma, will also be shown, and discussed.

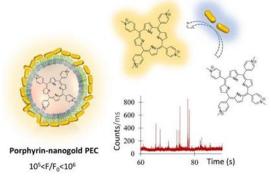


Figure 1. Microscale design towards fluorescence enhancement on porphyrin-nanogold PECs.

Keywords: Polyelectrolyte Microcapsules, Porphyrins, Gold Nanoparticles, Fluorescence Imaging, Plasmonic Antennas.

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# Development of inhalable mPEG-PLGA nanoparticles for lung cancer treatment

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Lung cancer has a high mortality rate among all common cancers [1]. Conventional lung cancer therapies are typically administered intravenously with low selectivity for tumor cells and serious side effects. The encapsulation of therapeutic proteins such as antibodies into nanoparticles for inhalable delivery is a promising strategy, which combines targeted and controlled drug delivery with the ability to protect protein structure and bioactivity. Moreover, antibodies are useful in treatment due to their higher specificity and bioactivity, and lower toxicity compared to small molecule drugs used in conventional therapy [2]. Still, the encapsulation of antibodies into nanoparticle for therapeutic purpose is a novel field, and new formulations have to be developed [3]. Thus, the aim of this work was the development and optimization of mPEG-PLGA nanoparticles formulated into dry powder by spray-drying aimed at lung cancer treatment. The optimized formulation was produced with 150 mg mPEG-PLGA and 1% Tween<sup>®</sup> 80, showing the lowest particle size of  $\approx$  300 nm, polydispersity index (PdI) of 0.36 and negative zeta potential of -24 mV, considered suitable features for antibody encapsulation. The spray drying optimization has demonstrated that D-mannitol and L-leucine were the best performing matrix excipients to obtain microparticles once their combination allows an increase in the yield due to leucine ability as dispersibility enhancer [4,5]. Microparticles resulting from their combination, present in the spraying dispersion at concentrations of 2% and 1% (w/v), respectively, were produced with spray-drying yields up to 59%, showing low powder adhesion to the apparatus. On the other hand, the other tested excipients, lactose, and D-trehalose resulted in hygroscopic powders with a sticky appearance. Further studies will focus on loading of therapeutic antibodies, aimed at establishing an inhalable lung cancer therapy.

Keywords: Inhalation; Dry powder; Lung cancer; mPEG-PLGA nanoparticle; spray-drying.

Acknowledgments: This work was funded by Fundação para a Ciência e a Tecnologia (FCT) in the scope of the projects UIDB/04326/2020, UIDP/04326/2020 and LA/P/0101/2020 of the Research Unit Center for Marine Sciences—CCMAR, and UIDB/04565/2020 and UIDP/04565/2020 of the Research Unit Institute for Bioengineering and Biosciences—iBB, and LA/P/0140/2020 of the Associate Laboratory Institute for Health and Bioeconomy—4HB. Cláudia Viegas would also to thank FCT for the PhD fellowship (2020.08839.BD).

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# A new type of biomass as support for paracetamol absortion

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In this work in a new type of biomass - insect exuviae have been made and used to assess the impact of different parameters such as the size of the particles, the temperature, for the absortion of paracetamol. Results and characterization (FTIR analysis and microscopic observations) are made to compare the different results and to explain the different behaviors of each sample.

Keywords: biomass, paracetamol, absortion



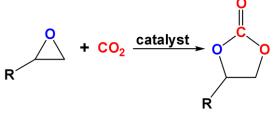
# Cyclic carbonates formation catalysed by a Iron(II) scorpionate.

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In terms of green metrics, direct coupling between  $CO_2$  and epoxides is one of the most attractive strategies for cyclic carbonate formation. this reaction as the advantage of being a 100 % atom economic transformation [1].



In this study, we aim to discuss the effect of reactionary parameters (pressure and temperature) on cyclic carbonate formation using styrene oxide, propylene oxide and cyclohexene oxide [2]. The differences in the catalytic activity and selectivity also will be presented.

Keywords: CO<sub>2</sub>, Scorpionate, Cyclic carbonates

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#### Acknowledgements

Funding from FCT (Fundação para a Ciência e a Tecnologia, Portugal) (UID/QUI/00100/2013, PTDC/QEQ-ERQ/1648/2014 and PTDC/QEQ-QIN/3967/2014 projects) are acknowledged.



# Pressurized liquids to obtain DHA enrich extracts from microalga Crypthecodinium cohnii

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Microalgae have emerged as a promising feedstock to produce biofuels and  $\omega$ -3 compounds, which have important applications in the food and pharmaceutical industry [1]. The marine microalgae *Crypthecodinium cohnii* (*C. cohnii*) is a non-photosynthetic heterotrophic dinoflagellate that can be found in tropical and temperate waters worldwide [2,3]. This oleaginous microorganism is capable of accumulating significant amounts of lipids (up to 50% of its dry weight), with a high fraction of docosahexaenoic acid (DHA), a polyunsaturated fatty acid (PUFA) of the  $\omega$ -3 group.

The present work aimed to explore the use of an environmentally friend technique, pressurized liquid extraction (PLE), to obtain lipids from C. cohnii and to implement a simple and environmentally friendly process for the co-production of biofuels and the high added-value product, DHA. Two solvents, considered green, were tested: ethanol and ethyl acetate. Ethanol is considered a GRAS solvent, being allowed for most of the food and pharmaceutical applications. Ethyl acetate is a bio-based solvent, with a wide range of applications in the food industry. With the purpose of optimizing the experimental extraction conditions for the maximum yield, an experimental design based on a surface response methodology, according to the Doehlert distribution for two factors, was built [4,5]. The evaluated factors were temperature (40-200 °C) and the time of extraction (2-20 min), being the response factors the yield in total fatty acids, in DHA and in fatty acids targeted to biofuel production. It was observed that the time of extraction was the most significant parameter in the process. Moreover, the yield of extraction increased with the temperature, as well as with the time of extraction. The isoresponse surface graphics allowed to determine the range of time and temperature in which the highest yield could be obtained. For the case of ethanol the maximum yield in total fatty acids was attained in the upper right quadrant of the graphic, corresponding to the highest temperatures and times of extraction. Finally, for DHA the highest yield was obtained in the right half of the graphic, which corresponds to all range of temperatures and the higher range of extraction time: 12-20 min.

Keywords: Pressurized Fluids, Microalga, DHA, Fatty Acids, Biofuels

# Acknowledgements

This work was financed by national funds through FCT - Fundação para a Ciência e a Tecnologia, I.P., within the scope of the project PTDC/EAM-AMB/30169/2017. The authors also thank FCT for financial support through the funding UIDB/00100/2020 and UIDP/00100/2020. Institute of Molecular Sciences is an Associate Laboratory funded by FCT through project LA/P/0056/202. Beatriz P. Nobre thanks IST and FCT for the Scientific Employment contract.

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# Challenges of Computational Dosimetry in Medical radiation physics applications

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The field of medical physics research using radiation cover mainly two areas, diagnostic and therapy. Diagnostic using X-ray and  $\gamma$  radiation is worldwide used routinely in several clinical tasks, such as X-ray breast imaging, CT and Positron Emission Tomography (PET) imaging. Cancer treatment using ionizing radiation (IR) plays an important role in the treatment of about 60% of cancer cases. Radiation dosimetry in diagnostic is mainly related with radiation protection purposes, being its assessment important for estimation of the incidence of stochastic processes in population submitted to this type of examinations. Radiation dosimetry is related to the estimation of deterministic effects and its accurate assessment is important to maximize the effectiveness of a specific treatment planning, both for external and internal beam irradiation techniques. In these two-radiation research areas (diagnostic and therapy) the use of computational dosimetry is an essential tool since continuously complement the clinical dosimetry in routine applications.

Specifically, the assessment of organ radiation doses is not directly possible. Operational quantities were introduced and defined by ICRU, which, together with conversion coefficients, can provide mean absorbed dose estimations. One the main research activity in computational dosimetry is related to the estimation of such as conversion factors that permit to link the operational quantities (e.g. air kerma) to organ-absorbed doses. In addition, computational modelling is often used to setup new radiation diagnostic/therapy techniques. In this Poster session some challenge examples in computational dosimetry will be reported, both in diagnostic and therapy applications. In this field, activities involving the IST groups are related to computational/experimental studies that permit both to optimize the existent clinical techniques (e.g. breast imaging) and to optimize and better understand new radiation therapies techniques (e.g. targeted radionuclide therapy and radio therapy with radio sensitizers).

**Keywords:** Computational dosimetry; Radiation medical physics; radiation therapy; radiation protection; Monte Carlo simulations;



# Structural and biological evaluation of chitosan-based scaffolds processed by gamma radiation for skin tissue engineering

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# BACKGROUND

Healing wounds continues to be an afflicting problem in multiple cases, such as in skin burns. Available options are limited, and frequently costly. Aiming to create biodegradable polymeric matrices to be used as skin scaffolds, chitosan based matrices were successfully prepared by gamma irradiation.

# METHODOLOGY

The preparation methodology involved the preparation of copolymeric solutions and their irradiation after freeze-dry cycles. Radiation doses up to 10 kGy were tested with a dose rate of 0.5 kGy/h. Chitosan of medium and low molecular weight, poly(vinylalcohol) (PVA), vinylpyrrolidone (VP) and gelatin were tested in order to optimize matrices properties. The developed chitosan based matrices were evaluated in terms of preparation methodology, composition, absorbed dose, structural and functional properties (FTIR, DSC/TGA, SEM, hydrophilicity, swelling in simulated physiological conditions and degradation in vitro), and in vitro biocompatibility using Human Caucasian Foetal Foreskin Fibroblasts (cellular viability, morphology and immunocytochemistry).

Scaffolds' effectiveness on the healing of wounds and skin regeneration/repair was evaluated by in vivo regeneration experiments in male Wistar rats.

# RESULTS

Materials and methods in use lead to matrices that are not cytotoxic to a human fibroblast cell line. Also, it was observed that Chitosan of low molecular weight and introduction of Gelatin revealed to be favorable to cellular growth leading to an improvement on cells' morphology and cytoskeletal organization

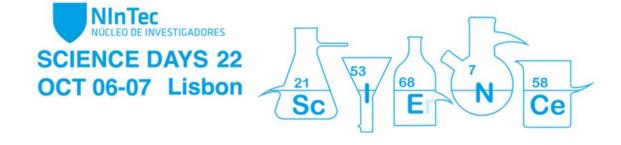
The best configuration ready for animal experiments was determined as being the one with a 2% content in low molecular chitosan and 5% in VP, prepared by gamma irradiation at 10 kGy after 2 freeze-dry cycles. The group of male Wistar rats where the matrices were applied, exhibited no signs of infection, a good tissue integration and an accelerated epithelization compared with the control group with no matrix. Histologically, the matrix implant site presented a simpler architectural organization than the normal tissues. Excluding keratinocytes, fibroblasts and new vessels were observed in the region.

# CONCLUSION

The developed matrices proved to be safe and biocompatible, promoting wound epithelization faster than left wound open for self-healing, filling in and closing up. Such matrices seem to be a promising alternative to the current options for the treatment of wounds and skin regeneration.

Keywords: chitosan: gamma radiation; cell proliferation; skin scaffolds, regenerative medicine





# October, 7 Oral Session

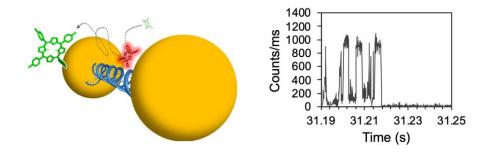


# Bringing light closer to molecules for a sensitive detection of disease biomarkers

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Fluorescence labelling is widely used for imaging or sensing applications and, for this purpose, strongly fluorescent dyes are available. Nevertheless, the performance of fluorescent molecules can be limited by low excitation rates, because the excitation cross section is typically smaller than the molecule's physical dimensions. This limitation can be overcome by using metal nanoparticles as optical antennas. Such approach has been explored to increase the sensitivity in fluorescence-based detection schemes [1], or to enable the detection of single-molecule fluorescence from weakly emitting molecules [2,3]. In this contribution, we will present our results on fluorescence enhancement by gold nanodimer antennas. Gold nanodimers were assembled from spherical gold particles using doubly-thiolated ds-DNA linkers to achieve narrow interparticle gaps. These assemblies are powerful antennas because of the large plasmon fields that can be generated at the nanogap hot-spots (figure 1).



**Figure 1:** (left) Scheme of a porphyrin molecule diffusing across the plasmon hot-spot of a gold nanodimer; (right) Emission time trace showing intense bursts of enhanced fluorescence from a single porphyrin molecule interacting with a gold nanodimer.

Keywords: Single molecule detection; Plasmonics; Fluorescence microscopy; Porphyrins; Biosensors.

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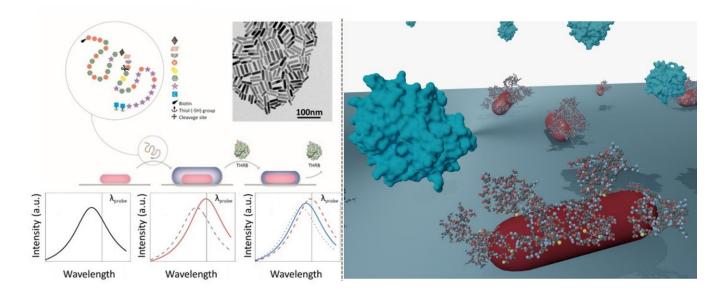
# A single-particle plasmon sensor to monitor proteolytic activity in real-time.

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Proteases are a subset of hydrolytic enzymes often involved in metabolic processes that ensure homeostasis. For diagnostic purposes, the concentration of proteases is commonly measured but due to its intricacies this is often misleading or erroneous, hence measuring proteolytic activity is more accurate and reliable. The current gold standard to determine the activity of proteases is based on fluorescent molecular rulers, such as FRET, which are sensitive to the environment and present limited photostability. Here, we established a label-free biosensor based on single gold nanorods that are functionalized with a design peptide that is specifically cleaved by thrombin. Through monitorization of plasmon shifts of many individual nanorods we determined thrombin's proteolytic activity in real-time. Our assay unveiled a couple of kinetic aspects that were compared and validated by a kinetic model that uncovered that plasmon shifts are dictated by a competition between peptide cleavage and thrombin binding, which have opposing effects on the measured plasmon shift. The sensor has a dynamic range of >2 orders of magnitude with a physiologically relevant detection limit of 3 nM. Plasmon-mediated label-free sensors open the window to a range of applications stretching from the diagnostics of bleeding disorders to fundamental proteolytic and pharmacological studies.



**Keywords:** Plasmonic nanoparticles, monitoring thrombin, proteolytic sensor, single-particle spectroscopy, kinetics.



# Supercritical Antisolvent precipitation: a path to nanocatalysts.

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Sustainability is a major topic these days, and catalysis gave, and is continuously giving, a great contribution to this. But catalysis is only truly sustainable if the paths we take to use it are sustainable in their own. An important aspect is the way catalysts are produced. In general, their production involves a multistep process that comprises several stages and operations, such as precipitation or other synthesis process, hydrothermal transformations, filtrations and washing steps, crushing and griding, and calcination or activation methods. To meet the principles of green chemistry1 and the goals of United Nations to sustainable development, the use of processes and methods that spend less resources and are likely to generate less waste should be selected and followed.

A possible way to follow in the catalysts' production is the supercritical environment. Nowadays, there are several processes that use supercritical fluids to generate micro and nanoparticles. One of them is the supercritical antisolvent precipitation. This technique is capable of precipitate micro or nano particles of catalysts or precursors, accordingly to the experimental conditions. The work developed in the last few years using supercritical fluids to producing catalysts, with this eco-friendly technique is now analysed in retrospective, considering benefits and disadvantages of the produced catalysts in this way.

Keywords: Supercritical fluids; Catalysts, nanoparticles; micronization

#### Acknowledgements

Support for this work was provided by FCT through UID/QUI/00100/2020.

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# Novel bio-based Gold nanoplatforms for cancer phototherapy

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Cancer is one of the leading health problems worldwide due to its mortality. In addition to conventional cancer therapies (surgery, radio-, chemo- and immune-therapies), other non-invasive therapies, with high precision and less side effects, have been studied in the last few decades such as photodynamic therapy (PDT) and photothermal therapy (PTT) [1,2]. The derivatization of the photoactive compound (photosensitizer, PS) with biomolecules such as carbohydrates allows a targeted delivery strategy by recognition of uniquely expressed or overexpressed receptors on tumor cells, thus, increasing the selectivity of the treatment [3]. The combination of PS derivatives with photothermal agents (i.e., Au nanoparticles) allows to simultaneously perform PDT (through formation of reactive oxygen species (ROS) from the cellular oxygen) with PTT, especially under hypoxia, since the slight increase in temperature induced by the photothermal effect results in a higher treatment efficiency [4,5].

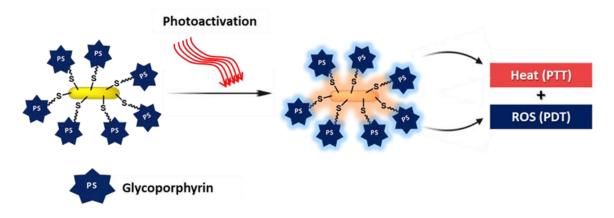


Figure 1. (Nano)formulation of bio-based AuNRs with glycoporphyrins

Keywords: Phototherapy; Glycoporphyrins; Gold nanorods; Cancer

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# High-performance instrumentation for diagnostics and control in fusion devices

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The ITER project demanding operating conditions, as well as other enabling experiments (including the recent fusion record breaking experiment - Joint European Torus) in relevant fusion projects, present new challenges to the diagnostics, control and instrumentation. The most critical requirements relate to the high acquisition rates (up to some gigasample per second), high physical event rate (up to several megaevents per second), need to handle enormous quantities of data in long experimental pulses (up to 30 minutes) and highly complex control and diagnostic algorithms. Radiation hardness of all equipment involved must also be taken into account for high magnetic fields as well as neutron irradiation in the fusion devices port cells.

The implementation of state-of-the-art designs was tested both with in-house built prototypes and complete systems installed in the major international fusion experiments. The main technologies used include Advanced Telecommunications Computing Architecture (ATCA), high speed electronic devices for signal digitization, complex real-time algorithms for physics analysis, control and data compression implemented in high-performance computing using field-programmable gate arrays and multicore processor architectures.

The control and data acquisition group at Instituto de Plasmas e Fusao Nuclear (Instituto Superior Técnico) in collaboration with LIBPhys-UC (Departamento de Física da Universidade de Coimbra) has conducted several projects and studies for the development of reliable high-performance processing tools and instrumentation for the diagnostics and control of fusion devices capable of complying with the most demanding requirements.

Keywords: Nuclear Fusion, High Performance Instrumentation, ITER Tokamak, JET Tokamak



# Radiation for Material, Environmental and Health Sciences Research at IRIS

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Ionizing radiation is used to modify physical, chemical and biological properties in different materials, which is the basis for many practical applications. In most cases, ionizing radiation processing is a clean technology with clear benefits for industry, public health and environment. All three ionizing radiation main sources commonly used in radiation processing (gamma, electrons and X-rays) are available at the ionizing radiation facility IRIS. Gamma irradiations are performed in an experimental cobalt-60 irradiator optimized for isotropic dose distribution at sample position. The linear electron accelerator (LINAC) available at IRIS delivers up to 10 MeV electron or photon beams (produced by electron/X-ray conversion). The facility is open to the scientific community and is mainly dedicated to the application of ionizing radiation technologies in RD&I in material, environmental and health domains. This presentation highlights the main aspects of an irradiation procedure and some examples will be presented.



Experimental gamma irradiator



Linear electron accelerator

**Keywords:** Radiation technologies, Biomedical applications, Advanced materials, Food safety, Wastewater treatment.



# Fleet of drones for radiological inspection, communication, and rescue

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The defence against Chemical, Biological, Radiological and Nuclear (CBRN) threats is an increasing demand due to wars, terrorist attacks, disasters or simply caused by negligence (e.g., decommissioned mines, medical waste). Drones, as well as advanced sensing technologies, play an important role in the increased protection of critical infrastructures and public spaces in the face of imminent threats of CBRN attacks. Radiological and nuclear threats, such as radiological dispersal devices ("dirty bombs"), nuclear power plant incidents, nuclear waste storage, mining sites, orphan sources and wars, namely, the actual Russia-Ukraine war, which are difficult to intercept and may release high levels of ionizing radiation, have a particular interest.

The project FRIENDS (Fleet of drones for radiological inspection, communication and rescue), with the collaboration of partners from IST (IPFN, ISR and C2TN) and from IT-Aveiro, and from different science domains, namely Electrical and Computer Engineering, Physics, Mathematics and Chemistry, aims design, develop and validate a fleet of drones equipped with navigation and radiological sensors for inspection and monitoring of scenarios with nuclear threats. In this project, a set of drone profiles are presented, being equipped with Light Detection And Ranging (LIDAR) to perform the cartography of the scenario and support real-time navigation, when combined with Global Navigation Satellite System (GNSS) and inertial measurement units, Red, green and blue (RGB) and RGB-depth (RGBD) cameras for image collection and support autonomous landing, and the radiological sensors Geiger-Muller counter (GMC) and Gamma Ray Spectrometer (GRS). These drone profiles are using in operations divided into three classes: 1) scouting for mapping the scenario with LIDAR and GNSS returning a 3D georeferenced map, 2) monitoring using the GMC and GNSS to provide a radiological intensity map and the estimation of the potential hotspots, and 3) inspection where the GRS is used to characterize the potential radionuclides present in the scenario.

Successful experiments were conducted in old mines of uranium ore supervised by the Portuguese Environment Agency (APA) and the Portuguese Mining Exploration Company (EDM).

Keywords: Nuclear Threats, Drones, Radiological Monitoring, Inspection and Mapping



# From Gravity to Gravity Waves: a Cursus Honorum

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My research started in General Relativity. A hamiltonian approach to black entropy was followed, where the entropies of various black hole solutions were obtained. The subprime crisis convinced me to move to fluid mechanics. Trapped modes in linear water-wave theory became my principle avenue of research. A brief stint in the History and Philosophy of Science came after the end of the postdoc. Presently my focus is in wave velocity and energy characterization for general non-linear solutions, in addition to implicit constitutive relations. Additional avenues of research are presented at the end.

Keywords: Gravity; Fluid Mechanics



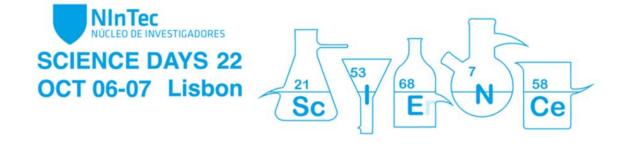
#### Quantum correlations: from quantum mechanical foundations to applications

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In this talk, I will introduce quantum correlations, one of the key aspects of quantum information theory, starting with the seminal example of Bell nonlocality. I will review Bell's theorem, which shows how quantum mechanics cannot be simulated classically. Generalizations of Bell nonlocality and other types of quantum correlations will be outlined. Experimental research and applications of quantum correlations will be briefly discussed, with a focus on quantum communication using quantum optics and light-matter interaction.





# October, 7 Round Table



# Round Table "The scientific employment: from University to the private sector"





Doutor José Vicente, Investigador do Instituto de Plasmas e Fusão Nuclear, Membro do Conselho Científico do Técnico, Membro da Direcção do NInTec

#### <u>Bio</u>

#### CONVIDADO

Professor Doutor Luís Ferreira, Reitor da Universidade de Lisboa

#### <u>Bio</u>

#### CONVIDADA

Professora Doutora Fátima Montemor, Vice-Presidente do IST e membro da Direção da IST-ID

#### <u>Bio</u>

#### CONVIDADA

Doutora Ana Margarida Ricardo, Investigadora do CERIS, membro do Conselho Geral da ULisboa e dirigente do SPGL/FENPROF

#### <u>Bio</u>

#### CONVIDADA

Doutora Sofia Aires Martins, Gestora de Ciência do iBB

#### <u>Bio</u>

# CONVIDADA

Doutora Maria Margarida Mateus, Supervisora de Investigação e Desenvolvimento na Secil

# <u>Bio</u>

# With the participation of the audience









