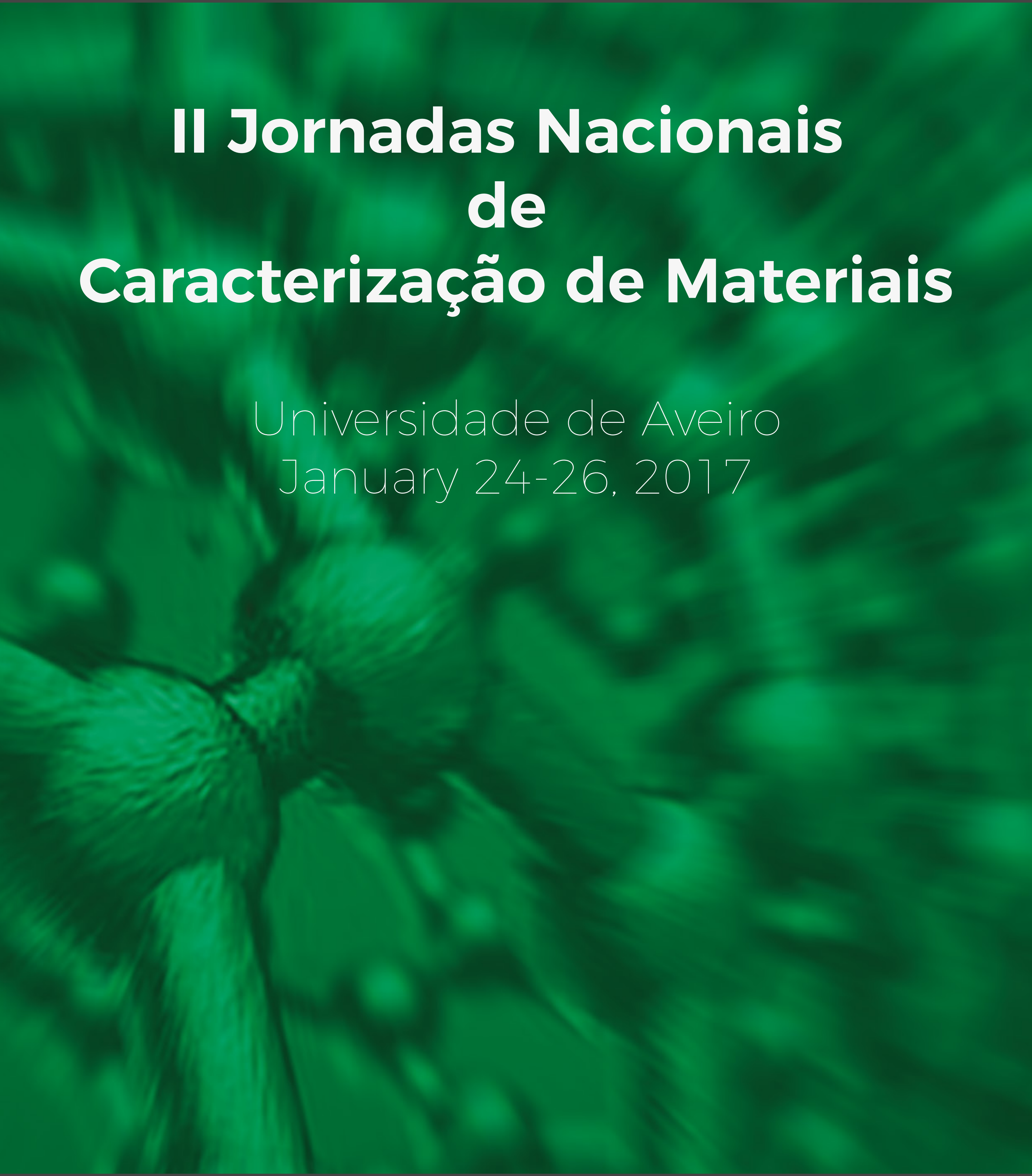

II Jornadas Nacionais de Caracterização de Materiais

Universidade de Aveiro
January 24-26, 2017

Book of Abstracts

Sponsors

Acknowledgements

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WELCOME MESSAGE

The world that surrounds us nowadays is made of incredible materials that have pushed our life quality and expectancy to levels never seen before over the last decades. Modern materials can be nano, functional, composite, smart/intelligent, or even a mix of these and are the building blocks of amazing technologies from which our society depend in a daily basis. Next generation materials promise to change the way the world is made. For example, a forever battery based on a nanotube-based battery could make rechargeable batteries last 20 times longer; scientists have now invented new polymer-based versions of superinsulating aerogels space suit stuffing some 500 times stronger than previous materials. Slippery liquid infused porous surfaces can cut friction in crude-oil pipes, halt ice formation on airplane wings or shed spray-painted graffiti from walls. Other fantastic examples of futuristic materials are plant plastics, flexible concrete, fireproof fatigues or cyber steel.

Despite of the enormous advancements and rapid progresses, the fundamental reasons behind the better performance or success of new materials often remains unknown. To better understand, tune and control the macroscopic properties of a material it is crucial to obtain an atomic/molecular level characterization using methods and tools that can direct the researcher towards new materials discovery pathways.

The development of new characterization methods by means of spectroscopy, microscopy and other analytical equipments is therefore of extraordinary importance to probe physical, mechanical, optical, electrical or chemical properties of these materials. The efficient use of such techniques is not only the cornerstone of the major achievements of a researcher working in academia but also key to a wide range of industrial processes, such as R&D support, interactive monitoring during production or quality control.

In this context the main goal of the workshop is to deliver a cross-disciplinary learning approach and condensed overview of major analytical techniques for the characterization of different types for materials with emphasis on practical applications. The workshop provides a series of plenary sessions followed by short courses, given by recognized experts, and will cover the "nuts and bolts" of the different characterization techniques. These presentations will be problem-solving oriented emphasizing case studies of relevance to industrial applications and are geared towards both novice and experienced scientists.

Participants are encouraged to submit an abstract for poster presentations aiming at sharing knowledge, promote collaborations and foster partnerships among the participants from academia and industry. The best-poster will be awarded at the closing ceremony.

The organizing committee welcome all of you.

COMMITTEES

Organizing Committee

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Joaquim Vieira
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Luís Carlos
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Augusto Lopes
CICECO, Depart. Materials & Ceramics Engineering, Univ. Aveiro, Portugal

Secretariat

Ruben Silva
CICECO, Univ. Aveiro, Portugal

Joana Moreira
PARALAB, Portugal

GENERAL INFORMATION

Registration

Registration includes:

- Admission to scientific sessions
- Coffee breaks
- Lunches
- Conference badge
- Participant kit (programme & digital version of the book of abstracts)

Poster and oral presentations (technical information)

Plenary sessions will have 60 minutes plus 15 additional ones for discussion.

All speakers should check with the Organization at least one hour prior to the beginning of their session to test and deliver the presentation.

The dimensions of the poster presentations should not exceed A0 (84 cm x 118 cm). Please note that the Organization will not be responsible for the posters that are left in the panels after the session.

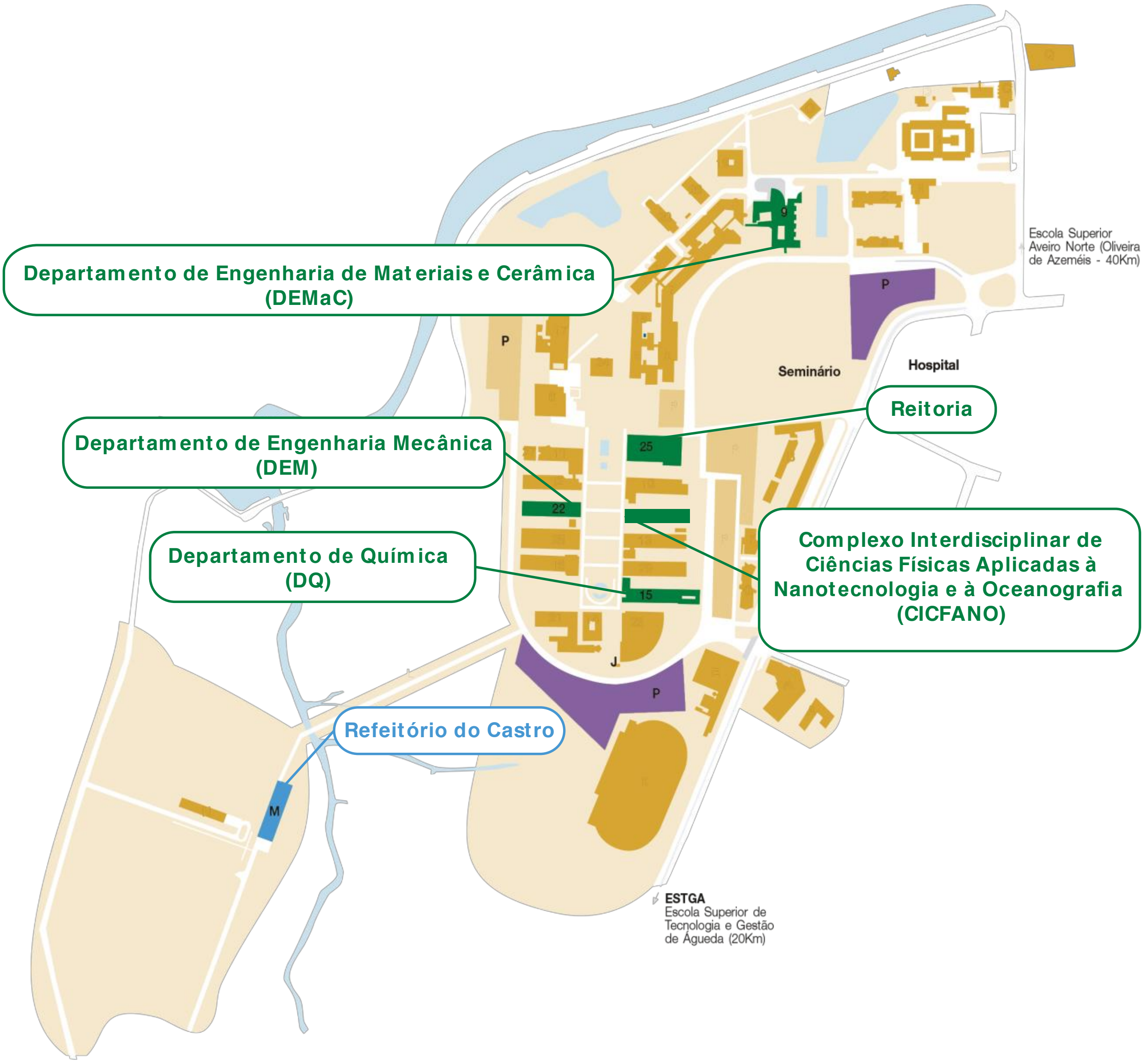
Official language

The official language of the Workshop is English. No simultaneous translation will be provided.

Badges and Security

It is essential that you wear your personal badge at all times while in the Workshop venue and during all the Events, as it is the official entrance pass to scientific sessions and other activities.

VENUE MAP


Departamento de Engenharia de Materiais e Cerâmica (DEMaC)
Departamento de Engenharia Mecânica (DEM)
Departamento de Química (DQ)
Refeitório do Castro
Reitoria
Complexo Interdisciplinar de Ciências Físicas Aplicadas à Nanotecnologia e à Oceanografia (CICFANO)
Escola Superior Aveiro Norte (Oliveira de Azeméis - 40Km)
Seminário
Hospital
ESTGA
Escola Superior de Tecnologia e Gestão de Águeda (20Km)
P
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Reach the university campus from Aveiro train station

Aveiro railway station is located at about 15 minutes walking distance or 5 minutes taxi ride from the University Campus or 10 minutes bus (line 4) which departs from outside the railway station.

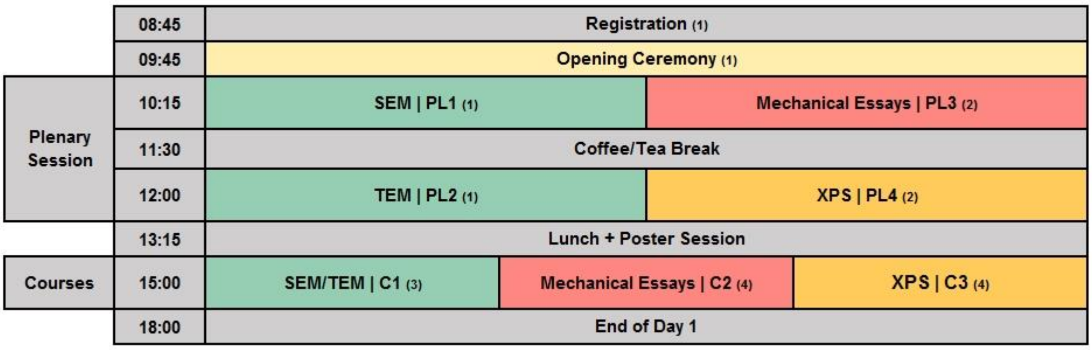
Reach the university campus by car

From the north using the A1 motorway or from the east using the A25: Take the A1 motorway headed to Lisbon. Exit the A1 in the direction of Aveiro and take the A25. There are two exits to the city from the A25, first "Aveiro-Norte" and some kilometers further on, the "Aveiro" exit. This second exit is the best for reaching the University of Aveiro campus.

From the south using the A1 motorway: Take the A1 motorway in the direction of Porto, exit the motorway at "Aveiro-Sul/Águeda" (exit 15) and follow the EN235 road directly to the University Campus. From the south, using the A8 and A17 motorways: Exit the motorway at "Aveiro-Sul" and follow the EN235 road directly to the University campus.

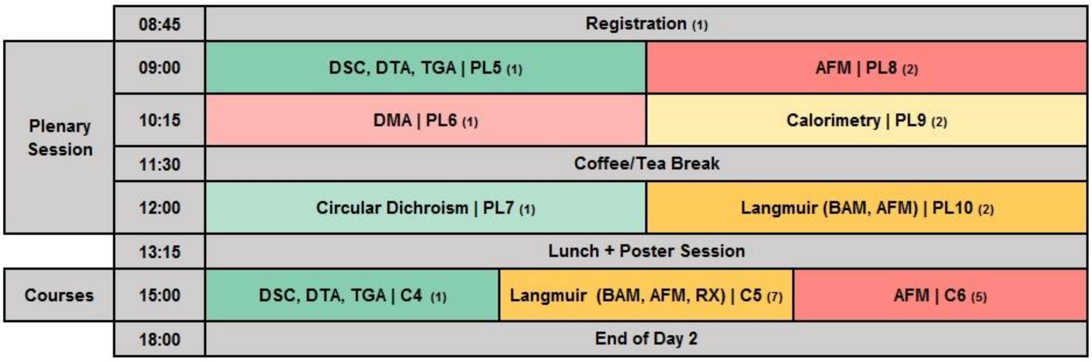
SCIENTIFIC PROGRAMME

Tuesday, 24 Jan



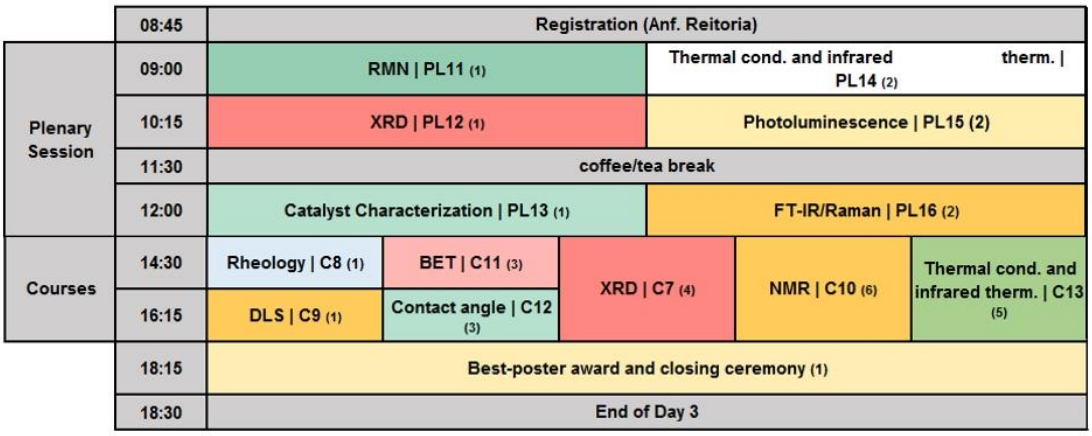
	08:45	Registration (1)		
	09:45	Opening Ceremony (1)		
Plenary Session	10:15	SEM | PL1 (1)	Mechanical Essays | PL3 (2)	
	11:30	Coffee/Tea Break		
	12:00	TEM | PL2 (1)	XPS | PL4 (2)	
	13:15	Lunch + Poster Session		
Courses	15:00	SEM/TEM | C1 (3)	Mechanical Essays | C2 (4)	XPS | C3 (4)
	18:00	End of Day 1		

Wednesday, 25 Jan



	08:45	Registration (1)		
Plenary Session	09:00	DSC, DTA, TGA | PL5 (1)	AFM | PL8 (2)	
	10:15	DMA | PL6 (1)	Calorimetry | PL9 (2)	
	11:30	Coffee/Tea Break		
	12:00	Circular Dichroism | PL7 (1)	Langmuir (BAM, AFM) | PL10 (2)	
	13:15	Lunch + Poster Session		
Courses	15:00	DSC, DTA, TGA | C4 (1)	Langmuir (BAM, AFM, RX) | C5 (7)	AFM | C6 (5)
	18:00	End of Day 2		

Thursday, 26 Jan



	08:45	Registration (Anf. Reitoria)				
Plenary Session	09:00	RMN | PL11 (1)	Thermal cond. and infrared therm. | PL14 (2)			
	10:15	XRD | PL12 (1)	Photoluminescence | PL15 (2)			
	11:30	coffee/tea break				
	12:00	Catalyst Characterization | PL13 (1)	FT-IR/Raman | PL16 (2)			
Courses	14:30	Rheology | C8 (1)	BET | C11 (3)	XRD | C7 (4)	NMR | C10 (6)	Thermal cond. and infrared therm. | C13 (5)
	16:15	DLS | C9 (1)	Contact angle | C12 (3)			
	18:15	Best-poster award and closing ceremony (1)				
	18:30	End of Day 3				

PLn = Plenary Session
Cn = Course
(1) = Anf. Reitoria
(2) = Sala Atos (Reitoria)
(3) = DEMaC
(4) = DEM
(5) = CICFANO
(6) = DQ
(7) = Sala Senado (Reitoria)

paralab

Paralab, being highly committed on its vision to contribute to a better and sustainable world by continuous investment in knowledge and science, associates again with the JNCM. After being the exclusive sponsor for the first edition in 2012, Paralab is now also backing the Best-Poster Award.

WHO WE ARE

We are one of the top suppliers of scientific and laboratory equipment in Portugal, representing the main brands for analytical and material characterization instrumentation

Past

- Founded in 1992 by post-graduation students from FEUP
- Background in automation
- Mastering a broad range of analytical techniques

Present

- Leading supplier for the main industries, universities and research centers
- Focus on after sale service
- Multidisciplinary and experienced team with engineers, chemists, pharmacists and biologists
- 15% of the team with PhD and 90% graduated
- Own applications lab

Future

- Consolidate leading position in Portugal
- Focus on international growth with offices in Barcelona, Madrid and Bilbao
- Internationalization allows Paralab to guarantee its sustainability and to establish as an Iberian reference with the power to attract benchmark representatives

WHAT WE DO

- Supply and service analytical and scientific equipments
- Services of technical consultancy, training and contract analysis
- Tailor made systems

WHY WORK WITH US

- Paralab, for its product portfolio and technical excellence of its team, ensures the best solution for each application and the best after sale service both on the implementation of the solution and supporting the instruments during its life time

Leading Analytical Solutions

INVITED SPEAKERS AND TUTORS

Plenary Sessions

PL1 / PL2 Scanning electron microscopy (SEM) & Transmission electron microscopy (TEM)

Pedro Tavares
Departamento de Química
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Augusto Lopes
Departamento de Engenharia de Materiais e Cerâmica
CICECO - Aveiro Institute of Materials
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Keyword: Electron microscopy

The electron microscopy (EM) is a very important tool in materials characterization, either for inorganic materials or for biological materials. To take full advantage of this powerful technique it is very important to understand the fundamentals of EM, the different types of electron microscopes and their main components, the basics of sample preparation and the features of image interpretation.

When a beam of electrons strikes a sample several types of interaction will occur. Transmitted electrons are the base of transmission electron microscopy (TEM) mode; secondary and backscattered are the base of scanning electron microscopy (SEM) mode. At the same time X-rays are also produced being used in energy dispersive spectroscopy (EDS), a technique that gives information about the local chemical composition of the sample [1,2]. In addition diffracted electrons can also be produced that can be used to characterize the local atomic structure of the sample [3].

Sample preparation for SEM or for TEM is a critical step for a successful study. For SEM analysis, the first decision is the choice between fracture or polished surfaces. In addition, electric conductive samples can be seen as is, but non-conductive samples must be surface coated with carbon or gold. Alternatively, low vacuum mode (up to 1.3 mbar) or environmental mode (up to 20 mbar) can be used for non-conductive samples or for hydrated samples. For TEM analysis, specific preparation techniques must be used for different types of samples, such as bulk materials, thin films, nanoparticles or biological materials.

References

[1] Joseph I. Goldstein, et al, *Scanning Electron Microscopy an X-Ray Microanalysis*, Kluwer Academic/Plenum Publishers, New York, 3rd ed., 2003.
[2] John J. Bozzola, Lonnie D. Russel, *Electron Microscopy*, Jones and Bartlett Publishers, Massachusetts, 2nd ed., 1999.
[3] D.B. Williams and C.B. Carter, *Transmission Electron Microscopy - A Textbook for Materials Science*, Plenum Press, New York, 2nd ed., 2009.

Short CV – Pedro Manuel de Melo Bandeira Tavares

Born: 13 September 1962, Aveiro, Portugal
Civil state: Married
Position: Associate Professor, Chemistry Department, Univ. Trás-os-Montes e Alto Douro, Vila Real, Portugal
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WebCV: http://www.degois.pt/visualizador/curriculum.jsp?key=4332872345666463

PhD in Chemistry, Univ. de Trás-os-Montes e Alto Douro, 2001.

Degree in Chemical Engineering, Univ. of Porto, 1985.

Teaching: Physical Chemistry, General Chemistry, Materials Characterization (Electronic Microscopy, X-ray diffraction).

Investigation Interests: Chemistry of materials, Oxide ceramics, Materials characterization, Electronic Microscopy, X-ray diffraction.

Publications: 128 articles with referee, 8 book chapters and 3 patents.

Participation in 21 investigation projects.

Selected Recent Publications with Electronic Microscopy (5):

Maria J. Lima, **Pedro B. Tavares**, Adrián M.T. Silva, Cláudia G. Silva, Joaquim L. Faria (2017) "Selective photocatalytic oxidation of benzyl alcohol to benzaldehydeby using metal-loaded g-C_3N_4 photocatalysts" Catalysis Today (in press), DOI: 10.1016/j.cattod.2016.11.023.

Rui S. Ribeiro, Adrián M.T. Silva, **Pedro B. Tavares**, José L. Figueiredo, Joaquim L. Faria, Helder T. Gomes (2017) "Hybrid magnetic graphitic nanocomposites for catalytic wet peroxide oxidation applications", Catalysis Today 280, p.184-191, doi: 10.1016/j.cattod.2016.04.040.

Nuno Cristelo, **Pedro Tavares**, Ernesto Lucas, Tiago Miranda, Daniel Oliveira (2016) "Quantitative and qualitative assessment of the amorphous phase of a Class F fly ash dissolved during alkali activation reactions – Effect of mechanical activation, solution concentration and temperature", Composites Part B, 103, pp. 1-14, DOI: 10.1016/j.compositesb.2016.08.001

Raquel O. Rodrigues, Manuel Bañobre-López, Juan Gallo, **Pedro B. Tavares**, Adrián M.T. Silva, Rui Lima, Helder T. Gomes (2016) "Haemocompatibility of Iron Oxide Nanoparticles Synthesized for Theranostic Applications: a High-Sensitivity Microfluidic Tool", Journal of Nanoparticle Research, 18: 194 (17 pp.) doi:10.1007/s11051-016-3498-7.

F. G. Figueiras, C. O. Amorim, J. Amaral, J. Agostinho Moreira, **P. B. Tavares**, E. Alves, V. S. Amaral (2016) "Magnetoelectric Effect Probe Through ppm Fe Doping in BaTiO3" Journal of Alloys and Compounds 661, 495-500, doi:10.1016/j.jallcom.2015.11.199

Short CV – Augusto Luís Barros Lopes

Born: 09 June 1964, Penafiel, Portugal
Position: Auxiliary Professor, Department of Materials and Ceramic Engineering, University of Aveiro, Portugal.
e-mail: augusto@utad.pt

PhD in Materials Science and Engineering, University of Aveiro, Portugal (2001).

Degree in Ceramic and Glass Engineering, University of Aveiro, Portugal (1989).

Teaching: Materials science and engineering, materials characterization techniques, structure and microstructure of materials.

Investigation interests: Electron microscopy and spectroscopy, microstructure, structure and properties of the materials, plastic deformation.

Publications: around 50 articles with referee.

Participation in 11 investigation projects.

Selected 5 recent publications with electron microscopy:

Juan Liao, Jose A. Sousa, Augusto B. Lopes, Xin Xue, Frédéric Barlat, António B. Pereira, Mechanical, microstructural behavior and modeling of dual phase steels under monotonic and complex deformation paths, Int. J. Plasticity (2016) (http://dx.doi.org/10.1016/j.ijplas.2016.03.010).

Alexandra Bintu, G.Vincze, Catalin R. Picu, Augusto B. Lopes, Jose J. Grácio and Frederic Barlat, Strain hardening rate sensitivity and strain rate sensitivity in TWIP steels, Materials Science & Engineering A 629, 54-59, (2015) (http://dx.doi.org/10.1016/j.msea.2015.01.080).

D. D. Khalyavin, A. N. Salak, A. B. Lopes, N. M. Olekhnovich, A. V. Pushkarev, Yu. V. Radyush, E. L.Fertman, V. A. Desnenko, A. V. Fedorchenko, P. Manuel, A. Feher, J. M. Vieira, and M. G. S. Ferreira, Magnetic structure of an incommensurate phase of La-doped BiFe0.5Sc0.5O3: Role of antisymmetric exchange interactions, Physical Review B, 92, 224428, (2015). (DOI: 10.1103/PhysRevB.92.224428)

Saeed Tamimi, João P. Correia, Augusto B. Lopes, Said Ahzia, Frederic Barlat and Jose J. Gracio, Asymmetric Rolling of Thin AA-5182 Sheets: Modelling and Experiments, Materials Science & Engineering A, 603, 150–159, (2014) (http://dx.doi.org/10.1016/j.msea.2014.02.048).

José J. Grácio, Catalin R. Picu, Gabriela Vincze, Nithin Mathew, Thomas Schubert, Augusto Lopes, Claudia Buchheim, Mechanical Behavior of Al-SiC Nanocomposites Produced by Ball Milling and Spark Plasma Sintering, Metall. Mater. Trans. A, 44,11, 5259-5269 (2013) (DOI: 10.1007/s11661-013-1874-9).

PL3 **Mechanical essays**

Mechanical properties of materials - from lab experiments to industrial applications

Gabriela Tamara Vincze
Centre for Mechanical Technology and Automation
Department of Mechanical Engineering
University of Aveiro
Campus Universitário de Santiago, 3810-193 Aveiro, Portugal
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In many important industrial applications, such as aerospace, automotive or packaging, economic and environmental concerns have driven the need of lighter but safer structures. Moreover, as a result a growing worldwide competitive market, manufactures are determined to reduce production costs. The environmental problems associated with the various steps in the life cycles of resources, materials and energy recovery determine a need to re-evaluate the ways in which natural resources are managed. Concerning the automotive industry, part of the overall strategy is to produce lower weight vehicles that mean increased performance, reduce fuel consumption and consequently fewer gas emissions to the environment. Therefore, the actual important issues as weight saving, improvement of passenger safety and better corrosion resistance has, in the last decades, raised the use of high-strength low alloy- carbon steel sheets and aluminium and its alloy sheets in the construction of vehicles in the last years. However, in many cases, while the strength is increased, the formability is penalized. The goal of materials scientists and engineers is to develop and improve materials with respect to given properties such as elastic modulus, strength, ductility, toughness, endurance and corrosion by a careful design of the microstructure. This can be achieved through the knowledge of the physical mechanisms influencing the mechanical properties of materials.

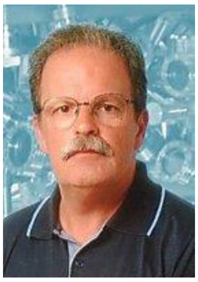
In this talk I will describe the basic mechanical properties of materials, with special attention to metallic materials. I will present results of our comprehensive research which focusses on linking the mechanical properties (i.e. macroscopic scale) with features that take place in material at microscopic scale and also with manufacture process. I will discuss the connection between modelling and simulation with experimental studies. I will show how this approach improves our understanding of the control of mechanical properties and thus leads to an improvement of mechanical behaviour.

Short CV

Gabriela Vincze received a PhD degree in Mechanical Engineering from the University of Aveiro Portugal in 2007. Currently she is an Invited Assistant Professor at the University of Aveiro. Her main research interests are the analysis of metallic materials (i.e. aluminium alloys, magnesium, steels, metal matrix composites, etc.) at different scales, the understanding of physical phenomena and the development of constitutive models to predict the mechanical behavior of materials for long-term applications in the area of plasticity. G. Vincze published more than 50 papers in high impact factor international peer review journals and international conferences proceedings. G. Vincze has well-established collaborations with top level research centers around the world. She was a key researcher in a cooperative international project between NSF and ESF and participated in 11 national research projects related to plasticity and forming applications. G. Vincze is a coordinator of Advanced Mechanical Engineering and Fracture Mechanics Group (GAME) of Centre for Mechanical Technology and Automation (TEMA), University of Aveiro. In the last thirteen years, G. Vincze taught courses on materials of mechanical construction, mechanical technology, advanced production technology, mechanics of solids, mechanics of structure, applied electronic instrumentation and experimental methods in mechanical engineering at the University of Aveiro.

PL4 X-ray photoelectron spectroscopy (XPS) - Fundamentals, methods and experimental opportunities

Fundamentals, methods and experimental opportunities



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CEMUP - Centro de Materiais da Universidade do Porto
E-mail: cmsa@cemup.up.pt

X-ray Photoelectron Spectroscopy (XPS) is an essential technique in modern materials science and technology offering experimental methods for the local analysis of the elemental composition of the outermost atomic layers of a solid (< 10 nm), under UHV experimental conditions.

The fundamental process of the technique is based on the photoelectric effect. The spectra of the kinetic energy distribution of the photoelectrons exited by monochromatic X-ray enable the measurement of the binding energy of the electrons in the solid, for very thin layer of material limited by the escape depth of the electrons with no kinetic energy loss.

Since the binding energy is the energy required to remove the electron from material and is specific to the orbital of the element of the excited atom, XPS can identify the elemental composition and relate peak intensity to the element atomic fraction in the analyzed thin layer. Additionally, detailed high resolution spectra can enable elemental peak shift measurement that correlate atomic chemical environment - chemical composition (oxidation state, chemical bonding).

This presentation will make a review of the fundamentals of XPS, basic experimental requirements and instrumentation, data acquisition and analysis methods and facilities.

Sample surface properties are an essential part of the XPS analytical experimental process, and the impact of conductivity, contamination, topography, heterogeneity (lateral and in depth) at the scale level of the analysis volume will be considered with detail.

The experimental opportunities and relevant data that XPS can provide will be considered from surface elemental analysis and chemical bonding characterization, to depth composition variation analysis (depth analysis by ARXPS and surface ion beam erosion) and lateral variation of composition analysis (mapping and imaging XPS).

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- J.F. Moulder, W.F. Stickle, P.E. Sobol and K.D. Bomben, Handbook of X-ray Photoelectron Spectroscopy, Perkin-Elmer Corp, 1992
- G. Beamson and D. Briggs, High Resolution XPS of Organic Polymers, John Wiley and Sons, 1992
- https://www.nist.gov/srd/nist-standard-reference-databases-surface-data
- http://www.casaxps.com/

Short CV

Carlos P. Moreira de Sá, born in 1952, has a Licence degree in Electronic and Digital Systems Engineering (1974, Faculty of Engineering of the University of Porto), and a Doctor degree in Electrical Engineering and Computers (1992, Faculty of Engineering of the University of Porto), and is presently a Senior Researcher of the Faculty of Engineering of the University of Porto, the Director of the Materials Centre of The University of Porto (CEMUP) and the Head of IMICROS – Image, Microstructure and Microanalysis Unit of CEMUP.

Carlos Sá started his career at the University of Porto in 1974 as a lecture assistant at the Faculty of Engineering of the University of Porto, and since 1981, as a researcher, he is involved in the implementation of the CEMUP project, as an infrastructure of the University of Porto for the support of research and development in the field of materials using adavanced experimental resources, and providing support and service to the departments and research centres and to other public or private research and industrial activities. In the course of this process he has completed his PhD thesis (1992) with a research project in the field of quantitative image analysis for materials microstructure characterisation.

In the frame of CEMUP project he took charge of the implementation, management and scientific and technical supervision of the first (1981) Laboratory for Scanning Electron Microscopy an X-ray Microanalysis (SEM/EDS), now in its third generation of equipment, of the Surface Analysis Laboratory (XPS/AES) (1991), now in its second generation of equipment, of the laboratory Quantitative Metallography (1997) and of the Laboratory for Scanning Probe Microscopy (SPM:AFM/AFM/MFM) (2007).

Carlos Sá has been deeply engaged, in some cases as a Principal Investigator, in all the research and infrastructure projects that have supported the build up and organization of the CEMUP.

Along this period he has provided extensive collaboration to the researchers from multiple scientific fields that make use of the experimental infrastructure the IMICROS - CEMUP (SEM/EDS, XPS, SPM, IA/QTM) in their research projects, he has regular collaboration in teaching of materials characterization methods and techniques in the frame of curricula of PhD and MSc courses of the University and he is responsible for regular training activities at CEMUP - Courses and Seminars on SEM/EDS, XPS and Image Analysis.

Fields of interest: high resolution methods for morphological, microanalytical and microstructutal materials characterization, namely Scanning Electron Microscopy (SEM), X-ray Spectroscopy (EDS), Electron Spectroscopy (XPS / AES) and Image Processing and Analysis.

PL5 Differential thermal analysis (DTA), Thermogravimetry (TGA) and differential scanning calorimetry (DSC)

Fundamentals, methods and experimental opportunities

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Fundamentals of high temperature thermodynamics and kinetics are reviewed shortly to emphasize the relevance of temperature dependence, and its relation with enthalpy changes or activation energies. Though the emphasis is mainly on solid state reactions and transformations of condensed phases, these processes often involve also gases (e.g. drying or solid-gas reactivity). Those fundamentals will also be extended to catalytic reactivity of gases, as exemplified by reforming reactions, partial oxidation of hydrocarbons, etc..

The main principles of detection of thermoanalyses are discussed, with main emphasis on exothermic/endothermic reactions, weight losses in solid/gas reactions or dilatometry to study thermochemical expansion and other temperature dependent dimensional changes. Still, one will also exemplify less common methods based on other properties with dependence on thermal schedule (e.g. electrical conductivity), as well as structural or spectroscopic changes (e.g. XRD, MS or FTIR with variable temperature).

The fundamentals of representative kinetic models for solid state reactions or transformations with variable temperature will be presented to emphasize the interdependence between different parameters of generic thermal schedules (temperature, time, heating/cooling rate). This will also be the basis to introduce widely used models of high temperature kinetics with variable temperature (Kissinger, Avrami-Nakamura,…), and to establish expected correlations between kinetic parameters under isothermal conditions and with variable temperature. These models also provide guidelines to seek optimised working conditions of thermal analyses, to extract the relevant kinetic parameters, and to attempt de-convolution of multi-step processes such as phase transformation involving nucleation and growth, partially overlapped steps of consecutive reactions, etc.

The basic principles will then be illustrated with representative study cases, starting from classical studies of phase transformations, crystallization of glasses and sintering, to more recent applications in different fields such as energy conversion (e.g. hydrogen storage and heat storage materials, conversion of hydrocarbons or biomass, etc.).

Short CV

Jorge Frade is a Professor of Material Science and Engineering at the University of Aveiro. He has graduated in chemical engineering (Coimbra, 1978), obtained his PhD from the University of Sheffield, UK (1983), and DSc/(Agregação) from the University of Aveiro (1995). Published about 300 SCI SCI papers in international SCI journals, with more than 5000 citations (h-index 39), and gave many talks at international conferences, (about 20 invited talks in the last 10 years). Received the prize for Scientific Excellence from the Portuguese Science Foundation (2004). Participates regularly in assessments of projects, individual grants (posdoc and PhD) and doctoral programs, and acts as a regular referee for a variety of international journals in materials science, electrochemistry, chemistry and related areas. Coordinated or was the Portuguese coordinator of 8 national projects and 8 international projects, and was also an active team member of many other projects.

His scientific interests are diversified, though with emphasis on solid state kinetics, thermodynamics and processing, materials for energy conversion, storage and management, and alternative emission lean technologies.

Powder processing includes solid state reactions, mechanochemistry, soft chemistry and other methods (combustion synthesis, freeze drying, hydrothermal synthesis,...). Ceramic processing is adjusted for specific microstructural and structural requirements, and for the impact on properties. This includes sintering under unusual conditions (reducing atmospheres) and less common firing schedules (e.g. 2-step sintering) and processing of highly porous ceramics with designed microstructures (cellular ceramics,..). Thermodynamic analysis is used to study interactions in multicomponent systems, to assess redox stability or reactivity with gases, and restrictions on solid state reactions. Kinetic models have been proposed for phase transformations and reactions in the solid state, with emphasis on models for variable temperature, to extract relevant kinetic parameters, and to assist the interpretation of transient responses obtained by other methods at high T (electrical conductivity, electrochemical titration).

Materials for energy conversion are mainly envisaged for: i) solid state electrochemical applications such as fuel cells and related systems (electrolytes, electrodes and catalysts), ii) mixed conducting membranes for oxygen separation or partial oxidation of hydrocarbons, and iii) materials for heat conversion and storage (PCM, thermoelectrics). The main emphasis is on enhancing required properties, overcoming critical limitations and designing materials with enhanced durability, tolerance to contaminants to enable conversion of low grade fuels, etc..

Interests in emission lean technologies are mainly focused on alternative electrolytic processes for CO2-lean steelmaking and to treat or recycle industrial residues, and more recently on emission-lean catalytic combustion.

PL6 Dynamic mechanical analysis (DMA)

Dynamic mechanical analysis and the characterization of materials: what can be done?

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In the last years, dynamic mechanical analysis (DMA) have been widespread used in the characterization of the mechanical/viscoelastic properties of materials for different kind of applications. It is a powerful technique widely used in the characterization of bulk materials where a small sinusoidal stress is applied to the sample being the resulting displacement measured. Through this technique, it is possible to determine the stiffness and damping characteristics of a material with respect to temperature, frequency or time, stress, atmosphere or a combination of these parameters. DMA is particularly important for materials that exhibit a viscoelastic behavior which is crucial to the knowledge of their solid-state rheological performance in the prediction of their mechanical performance in a real service situation. Indeed, a proper mechanical characterization is among the most important physical tests that must be carried out. In addition to the characterization of bulk properties directly affecting material performance, DMA also supply information about major transitions of the materials, as well as secondary and tertiary transitions not readily identifiable by other methods. DMA equipment also enables studies in different mechanical configurations such as in tensile, flexural, compression or shear modes, depending in the geometrical shape of the samples. More importantly, when performing DMA, it is primordial to recreate the environment that the material will face once, drastic differences in the material properties can be obtained depending on the experimental conditions. DMA allows investigating material properties of a wide range of research areas such as, detection and characterization of relaxation processes [1-3], measurement of the modulus and damping [3, 4], physical ageing, interface behaviour in composites and immiscible blends [5], crosslinked materials and compatible multi-component systems. Several examples will be presented, mainly involving the characterization of materials for medical applications, including unconventional tests that can be performed through DMA.

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Short CV

Sofia G. Caridade received her MSc in Materials Engineering in 2007 from the University of Minho. Her master work was performed in the *3B's research group, Biomaterials, Biodegradables and Biomimetics*. She has received an award for her master thesis by the Order of Engineers in 2008. In 2013, she received her PhD in Materials Engineering by the same institution with the thesis entitled "Bioactive membranes for bone regeneration". From 2013 to 2016 she worked as a postdoctoral researcher at the 3B's research group and, nowadays she is a postdoctoral fellow at CICECO, University of Aveiro. She has 48 papers and 1 book chapter and she has been acting as referee of several international peer-reviewed journals upon invitation. Her current research interests include materials science, biotechnology, biomaterials, development of materials and membranes for controlled drug delivery systems, study of viscoelastic properties and glass transition and characterization of porous systems for tissue engineering.

PL7 Circular dichroism

Circular dichroism: fundaments and applications

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Keywords: circular dichroism; coordination compounds; chiral complexes; protein-metal binding; DNA-metal binding; protein secondary structure.

Circular dichroism (CD) is a widely applied spectroscopic technique very useful in the study of both biological and non-biological systems. It is also an invaluable tool in inorganic chemistry, particularly in coordination chemistry. The fundamentals of the technique will be explained and applications in the following fields will be described: i) how CD may be used empirically to obtain structural and analytical information on transition metal complexes with optically active ligands; ii) information on the interaction of metal ions with large bio-molecules such as proteins and DNA and iii) protein secondary structure determination.

Short CV

Isabel Correia graduated in 1997 in Chemical Engineering at Instituto Superior Técnico, and completed her Ph.D. in 2003 also in Instituto Superior Técnico, under the supervision of Prof. João Costa Pessoa. Her Ph.D. thesis focused on the development of potentially therapeutically active coordination compounds. From 2003 to 2008 she did postdoctoral studies in several universities in Europe: TuDelft in the group of Prof. Roger Sheldon, in which she studied the application of biocatalysts in green oxidation reactions; Centro de Química Estrutural, with Prof. João Costa Pessoa, where she studied the application of transition metal complexes in green oxidations, and in Imperial College, in the group of Prof. Tom Welton, where she evaluated the reactivity of transition metal complexes in ionic liquids.

In 2008 she received an assistant researcher position under the Ciência 2007 program to develop her research in Centro de Química Estrutural and in 2013 a principal researcher position under the Investigador FCT program to work in the same research institution. She has been awarded the scientific direction of two FCT projects: POCI/QUI/55985/2004 (Synthesis, structure and reactivity of transition metal complexes with potential application in oxidative catalysis) and PTDC/Qui-Qui/098516/2008 (Reactivity of transition metal complexes in ionic liquids).

She co-authored 62 publications, 1 book chapter, 2 proceedings with scientific refereeing, 7 conference proceedings and 93 technical presentations (14 as speaker) at national and international conferences. Her current H index is 20 and her publications have 1188 citations. Currently she is supervising the research of 2 master and 2 PhD students.

Her research interests are in the filed of development of coordination complexes for application as therapeutic agents; DNA binding studies of metal complexes; determination of the secondary structure of proteins by circular dichroism; evaluation of the binding of transition metal ions to proteins; development of biocatalysts and coordination complexes for sustainable oxidation reactions; and evaluation of the structure and reactivity of transition metal complexes in ionic liquids.

PL8 Atomic force microscopy (AFM)

Circular dichroism: fundaments and applications

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Since its invention in 1986, atomic force microscopy (AFM) has become a major instrument in nanoscale science and technology. AFM is a microscopic technique for imaging a surface topography by using attractive and repulsive interaction forces between atoms constituting a tip end on a flexible cantilever and a sample. It was almost immediately realized that AFM could be extended to map forces of different types, such as magnetic and electrostatic forces, as well as for probing chemical interactions. Dual capability of probing forces and currents using AFM has led to rapid growth of a variety of Scanning Probe Microscopy (SPM) techniques such as Magnetic Force Microscopy (MFM), Electric Force Microscopy (EFM), Kelvin Probe Force Microscopy (KPFM), Conductive Atomic Force Microscopy (c-AFM), Piezoresponse Force Microscopy (PFM) and others. They provide unique capability to access local electric, magnetic, mechanical, electromechanical, optical and thermal properties of materials on the nanometer scale. It has been demonstrated that AFM-SPM approach provide not only imaging capability but also control and modification of the local structure and material functionality at the nanoscale. In this lecture, major AFM and SPM modes will be shortly described and their applications to a wide range of materials will be presented. It will be shown that Piezoresponse Force Microscopy as applied to ferroelectric and ionic conductor materials is indispensable for studying fundamental phenomena and can be very helpful in solving various application problems. Finally, several examples of using AFM-SPM in materials science will be presented.

Short CV

Andrei Kholkin has received his M.Sc. degree in Physics from Leningrad State University and Ph.D. degree in Solid State Physics from A. F. Ioffe Physical-Technical Institute of the Russian Academy of Sciences. Until 1993 he has been a research staff member of the Laboratory of Ferroelectricity and Magnetism at A. F. Ioffe Institute where he studied kinetic phenomena in ferroelectrics and high-temperature superconductors including ferroelectric field effect. Since 1993, he has been working outside Russia and held several research positions at Leibniz Institute for Solid State and Materials Research (Germany), Swiss Federal Institute of Technology (Switzerland) and Rutgers University (USA). He is currently a research coordinator and head of functional imaging and nanomaterials of CICECO - Aveiro Instititute of Materials, Aveiro (Portugal). His group develops novel multifunctional materials (including ferroelectrics, multiferroics, biomaterials, and ionic conductors) and scanning probe microscopy techniques such as Piezoresponse Force Microscopy and Electrochemical Strain Microscopy for their study. His current research interests spans from multiferroics (bismuth ferrite and magnetoelectric composites) to ferroelectric biomaterials and to graphene/graphene oxide.

He co-authored over 400 technical papers (H-index 42) in the area of functional materials including numerous reviews and book chapters. He was a coordinator of three European projects on multifunctional materials and coordinated many national and bilateral programs. He currently serves as an Associate Editor-in-Chief for the IEEE Transactions on Ultrasonics, Ferroelectrics and Frequency Control. He is a member of editorial boards of several scientific journals and serves in advisory boards of international conferences on ferroelectrics. He was a guest editor of four Focused Issues of Journal of Applied Physics (2010-2013), Special Issue of MRS Bulletin on Nanoelectromechanics (2009), Special Issues of Ferroelectrics and Transactions on Ultrasonics, Ferroelectrics and Frequency Control (2006-2007, 2012)

During last several years he was a co-chair of Technical Program Committees of the Joint IEEE UFFC Symposia (Singapore, 2015, Czech Republic, 2013), general chair of the 22nd IEEE ISAF-ECAPD-PFM conference (Portugal, 2012), general co-chair of the 21th IEEE ISAF conference (Canada, 2011), and general chair of the 6th and 11th European Conferences on Applications of Polar Dielectrics (ECAPD). Also, he was a co-founder of the new conference series “Piezoresponse Force Microscopy and Nanoscale Phenomena in Polar Materials (PFM)” started in 2009 in Portugal and continued in Japan, Canada, China, Czech Republic, Russia, Singapore, and Germany.

Dr. Kholkin is a member of the Ferroelectric Standing Committee and Ferroelectric Web Editor of IEEE. He was a recipient of the “Excellency” award from the Portuguese Foundation for Science and Technology (FCT). Dr. Kholkin was awarded by the title of IEEE Fellow in 2012 *“for contributions to electromechanical characterization methods and applications"*. He also received a Ferroelectric Recognition award of IEEE in 2015.

Dr. Kholkin was a visiting professor/researcher in a number of research organizations and Universities: Shonan Institute of Technology (Japan), Materials Science Institute (Spain), Prince of Songkla University (Thailand), Institute of Physics (Latvia), University of Limerick (Ireland), University of Oulu (Finland), Université de Valenciennes, Université de Picardie Jules Vernes, Ecole Centrale Paris (France), University of São Paulo (Brazil), and Ural Federal University (Russia).

PL9 Calorimetry

Calorimetry, microcalorimetry and scanning calorimetry. How does it work? What can we measure?

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Calorimetry is the science associated with determining the changes in energy of a system by measuring the heat exchanged with the surroundings. That sounds scientifically quite obvious, low tech and low fashion. In fact most students likely do not remember using such a *fancy piece of equipment* known as a calorimeter. The reason for this lack of memory, is because the calorimeter used in science labs is more commonly referred to as simple Dewar vessel or Styrofoam cup, identical to those we have at home. The more sophisticated models include a lid on the vessel with an inserted thermometer and maybe even a stirrer. Additionally, the experimental results are often unclear, badly understood and a mess in the interpretation of the process under study, time and temperature.

In fact, calorimetry, microcalorimetry or scanning calorimetry is a set of powerful experimental tools that have been successfully used in many fields of science. The information we can extract from the changes in energy of a system gives us some unique insights concerning the processes and transformations.

Calorimetry is used to measure the heat flow associated with physical and chemical transformations. The heat flow can be used as a transducer to measure/identify, phase change, equilibrium, chemical and physical kinetics, etc.

In this lecture I will try to explain how calorimetry works and can be used and the difference between calorimetry, microcalorimetry and scanning calorimetry. I will describe and present some examples concerning what can we measure and try to convince you how sophisticated and elegant calorimetry can be. [1-3]

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Short CV

Bachelor in Chemistry (UPORTO, 1987) and PhD. in Chemistry (Physical Chemistry) (UPORTO, 1996), Associate Professor, Faculty of Sciences of the University of Porto, Department of Chemistry and Biochemistry. Presently is the Director of the First Degree in Chemistry. Coordinator / member of R&D projects. Leader of the NSO-Nanostructures & Self-Organization Group. Co-Editor of two international journals in the field of Thermophysics Evaluator in the FCT evaluation panels. Co-Author of Two National Patents. The research area is Chemistry - Physics: Experimental Methodologies; Calorimetry; Molecular Thermodynamics; Thermophysical Properties; Thin Film fabrication and characterization; Organic semiconductor materials; Ionic Liquids. Co-author of more than 150 scientific articles in the field of chemistry-physics, physicochemistry, chemical engineering, material chemistry.

PL10 Filmes de Langmuir/Langmuir-Blodgett, Balança de Langmuir e caracterização (BAM, AFM, RX)

Chains @ interfaces - Langmuir and Langmuir-Blodgett films of molecular and ionic species

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Langmuir films are 2D supramolecular structures of amphiphiles, which form at the air-water interface. Depending on the type of surfactant, the ranges of surface pressure and temperature, Langmuir films can adopt different phases, exhibiting a variety of structures and organize into monolayers, bilayers and multilayers.

Often, Langmuir films can be transferred to the surface of solid substrates without losing their original organization forming Langmuir-Blodgett films.

In this presentation the basic principles of Langmuir film formation, their characterization and applications will be presented. A number of case studies will be presented and discussed involving several types of amphiphiles such as fluorinated surfactants, “primitive surfactants” and long chained ionic liquids.

Short CV

Eduardo J. M. Filipe got a degree in Chemistry at Faculdade de Ciências da Universidade de Lisboa and a PhD in Chemistry at Instituto Superior Técnico in the area of cryogenic fluids. He teaches at the Chemical Engineering Department of IST since 1987. He taught as invited Professor at Université Renée Decartes – Paris V (France) and worked as visiting researcher at the University of Vanderbilt (USA), Sheffield University (UK), Imperial College (UK) and Université Pierre et Marie Curie (France).

His research interests range from the development of new nano-structured materials and biocompatible fluids (respiratory emulsions and blood subtitutes), the properties and structure of complex fluids and their interfaces, to systems relevant to the oil industry (alphaltene stabilization and phase equilibria) and carbon capture. The systems under study often involve perfluorinated substances and ionic liquids and the adopted strategy combines a diversity of experimental measurements, computer simulation and theoretical modeling.

PL11 Nuclear magnetic resonance (NMR)

Nuclear magnetic resonance (NMR)

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Keywords: Solid-state NMR spectroscopy; magnetic fields; intermolecular interactions; crystalline/amorphous materials

How can humans communicate with invisible subatomic magnets through radio waves and “see” a response from such invisible entities? And how can we use it to extract useful chemical/structural information to understand solid matter?

This talk intends to provide answers to these questions providing to the audience a primer to the basics of the solid-state NMR (ssNMR) ‘*multiverse’* and a selection of case studies, including examples relevant to industrial applications.

The eight Nobel prizes associated to the NMR technique spanning over more than 70 years of research clearly show its importance and the continuous interest revealed by scientists to further develop the technique. Over the last decades, the number of studies exploiting ssNMR to solve solid-state chemistry problems has vastly increased showing the exquisite sensitivity of NMR to probe local chemical environments, sense local dynamics and identify intermolecular interactions (*e.g.*, hydrogen bonds, CH···π, π···π), which are the building blocks of all the strange properties of the matter that surrounds us.

This presentation is targeted to non-specialists of the technique and will start by addressing the NMR physical phenomenon with a pictorial explanation of the main ssNMR concepts; followed by a series of selected ssNMR applications aiming at illustrating how to extract atomic level structural details from industrially relevant crystalline and amorphous solids (*e.g.*, pharmaceuticals, heterogeneous catalysts, porous sorbents, energy-related materials.) to help in better understanding macroscopic properties of materials.

Short CV

Luís Mafra. b 1978, is currently a Principal Researcher and Manager of the Solid-state NMR (ssNMR) facility at CICECO - Aveiro Institute of Materials, University of Aveiro. Got his BSc/MSc degree at Universidade Nova de Lisboa in 2003. In 2006 he obtained a dual PhD degree from University of Caen (LCS), France & University of Aveiro, Portugal, working on ssNMR spectroscopy. During his PhD he developed NMR methodology to study materials, mostly using 1H CRAMPS NMR techniques and methods to observe quadrupolar nuclei. In 2007, he joined CICECO - Aveiro Institute of Materials as Assistant Researcher and manager of the ssNMR unit. In 2011, Invited Researcher, Max-Planck-Institut für Polymerforschung, Mainz, Germany. Luís Mafra has received various invitations, honors & awards recognizing his career achievements: 2014, promoted to Principal Researcher at CICECO under the national "Investigador FCT" competitive program. 2014, Adjunct Senior Lecturer honorary title, Sydney University (Australia). 2012, guest scientist, University of Oviedo, (Spain) with a research excellence fellowship (Futtalent program). 2006, recipient of Celestino da Costa/Jean Perrin prize. 2009, António Xavier Bruker prize. His current research interests include the combination of advanced ssNMR techniques with XRD and computational methods to study the intermolecular interactions of small molecules (pharmaceuticals) and porous materials relevant for catalysis and gas capture applications. He contributed with about ~26 talks and ~17 invited talks at international conferences; 17 invited oral presentations in research centres overseas. Published ~70 peer-reviewed full papers listed at the SCI (> 40% found in journals with IF > 5) and 5 book chapters related to ssNMR. He is also a member of the editorial board of the solid-state NMR journal (Elsevier); regular reviewer of several Elsevier, Wiley, RSC and ACS journals; reviewer of projects from governmental funding agencies and since 2010, he has been deeply involved in technology transfer and collaborative research with multiple private companies.

PL12 **X-ray diffraction (XRD)**

X-Ray Diffraction – Theory and Practice

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This lecture will feature a brief introduction to the theory of X-Ray Diffraction and an overview of different techniques of XRD that can be used to study various type of samples: single-crystals, polycrystalline (PXRD), thin-films (grazing incidence XRD and X-ray reflectometry) and materials featuring only short-range order (SAXS). Practical details on sample preparation and instrumentation will also be addressed.

Short CV

Full professor at Physics Department, University of Coimbra (UC). Coordinator of the Condensed Matter Physics thematic research line at CFisUC. Has authored or co-authored more than 275 publications in the ISI Web of Science, mainly in the fields of condensed-matter physics, chemical-physics and chemical crystallography. Director of the X-ray Research Centre for Materials Research (UC) from 2007-2015. Visiting scientist at the European Synchrotron Radiation Facility (2000-2001), has acted as member of the proposal evaluation panels, Scientific Advisory Committee and Council of this facility. Has been vice-president of the Scientific Council of the FCTUC, vice-director of the UC Institute for Interdisciplinary Research, and is currently the Director of the scientific council of the Physics Department at UC and Vice-President of the Portuguese Physical Society.

PL13 Catalyst characterization

Catalyst Characterization

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In heterogeneous catalysis, reactants and catalyst are in different phases; most often, the catalyst will be a solid porous material, in order to maximize the surface area in contact with the reactants. Industrial solid catalysts can be of two types: massive catalysts, consisting entirely of active substances; and supported catalysts, consisting of active substances dispersed on a support, or carrier. In general, the support is inert, although in some cases it might present activity on its own (eg, bifunctional catalysts). The active components of the catalyst may be metals, non-stoichiometric metal oxides (or sulfides) and stoichiometric oxides with acidic properties (solid acids). The activity of the catalyst will be determined by the presence of suitable active sites, capable of chemisorbing the reactants and forming surface intermediate species of adequate strength. However, these sites must be accessible to the reactants. Thus, the characterization of a porous catalyst will include both its textural characterization (total surface area, porosity and pore size distribution) and the characterization of the active sites. After a short overview of the methods available for textural characterization, we will focus our attention on the characterization of the active sites. As an example, we will consider the case of a supported metal catalyst, and will show how to determine the active metal surface area, and how to calculate the “metal dispersion”, defined as the fraction of exposed metal atoms. Methods include selective chemisorption, TEM and XRD. Characterization methods for oxide and acid catalysts will be briefly discussed.

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Short CV

José Luís C. C. Figueiredo (PhD, Imperial College, London, UK, 1975) is Professor Emeritus at the Chemical Engineering Department, Faculty of Engineering, University of Porto, Portugal, and Director of the Laboratory of Catalysis and Materials (LCM), Associate Laboratory LSRE-LCM. Most of his research has been focused in the areas of Carbon Materials and Heterogeneous Catalysis. He is a Member of the Editorial Boards of the journals CARBON (Elsevier), Fuel Processing Technology (Elsevier), and Periodica Polytechnica – Chemical Engineering (Budapest University of Technology and Economics). He is also a Member of the Academy of Sciences of Lisbon. Among others, he has received the following Scientific Awards: *Award for Scientific Excellence*, Ministry for Science and Higher Education, 2004; *Lee Hsun Research Award on Materials Science*, Institute of Metal Research, Chinese Academy of Sciences, 2014; *Ferreira da Silva 2014 Prize*, Sociedade Portuguesa de Química, SPQ (Portuguese Chemical Society).

Published 8 books (as author or editor), and co-authored 2 patents, more than 270 scientific papers in peer-reviewed journals, and more than 40 book chapters.

H index = 54; Citations: > 10,400 (SCOPUS, accessed on 13/01/2017).

The paper *Modification of the surface chemistry of activated carbons*, J.L. Figueiredo, M.F.R. Pereira, M.M.A. Freitas, J.J.M. Órfão, CARBON, **37** (1999) 1379-1389, is one of the most cited Portuguese papers in the field of Chemistry (1534 citations in SCOPUS, accessed on 13/01/2017).

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PL14 Thermal conductivity and infrared thermography

Thermal conductivity and infrared thermography

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Keywords: Thermal conductivity, infrared thermography, heat diffusivity

Thermal issues pose the need and challenge to perform experimental studies, from materials properties to kinetic thermal processes that occur above and below room temperature, with increasing demanding capabilities, down to the sub-micron length scale and millisecond time scale. Also, thermal processes are a useful partner as a non-destructive technique to assess materials and industrial processes.

The diversity of the problems and situations in I&DT activities and also on predictive maintenance is considerable. The application and impact of both techniques/studies on energy efficiency, refrigeration, systems performance, health and comfort as well as related industrial applications will be presented.

Short CV

Vitor Amaral was born in 1962 and obtained his PhD in Condensed Matter Physics at the University of Porto in 1993 and is presently Professor Catedrático (2009) at the Physics Department of the University of Aveiro. His main research interests have been related to magnetism and multiferroic phenomena in complex oxides, thin films and nanoparticles and on the application of nuclear solid state techniques. Recent topics are magnetothermal, and magnetostructural effects and their applications in refrigeration and thermal management processes.

He is a researcher at Laboratório Associado CICECO "Aveiro Institute of Materials", being the coordinator of Group 2. "Multifunctional Ferroic Ceramics and Nanostructures" and also at ISOLDE-CERN (Switzerland), where he coordinates projects on the application of radioactive isotopes for hyperfine studies on graphene, magnetic and multiferroic materials.

He is author/co-author of more than 219 scientific publications (ORCID), 198 in SCI index and 1 patent.

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PL15 **Photoluminescence**

Luminescence and Its Applications

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Keywords: photoluminescence; solid state lighting, random lasers, thermometry

Luminescence is a general term that describes any non-thermal processes in which energy is emitted in the ultraviolet, visible or infrared spectral regions from electronically excited species. The term broadly includes the commonly-used categories of fluorescence and phosphorescence. Fluorescence occurs where emission ceases almost immediately after withdrawal of the exciting source, whereas in phosphorescence the emission persists for some time after removal of that excitation. The distinction between the so-called types of luminescence specifies the activating energy as a descriptive prefix. For instance, Bioluminescence is related with light emission from lived animals and plants, Cathodoluminescence results from excitation by electrons, Chemicaluminescence is the emission occurring during a chemical reaction, Roentgenoluminescence is produced by X-rays, Triboluminescence is ascribed to rubbing, mechanical action, and fracture, Electroluminescence is the conversion of electrical energy into light, and Photoluminescence results from excitation by photons.

The lecture will present fundamental aspects behind photo and electroluminescence discussing specific applications and devices, such as LEDs, luminescent solar concentrators, random lasers and luminescent thermometers [1,2].

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Short CV

Luís António Dias Carlos got his Ph.D. in physics from the University of Évora, Portugal, in 1995 working on photoluminescence of polymer electrolytes incorporating lanthanide salts. Currently, he is Full Professor in the Department of Physics at the University of Aveiro and vice-director of the CICECO-Aveiro Institute of Materials (Portugal). He is member of the Lisbon Academy of Sciences and of the Brazilian Academy of Sciences. His current research interests include luminescent nanothermometers, luminescent solar concentrators, organic-inorganic hybrids for green photonics (solid-state lighting and integrated optics), and luminescent/magnetic nanoparticles, as new probes for multimodal imaging. He has published around 390 papers and 6 international patents, which have received ca. 12000 citations (Hirsch' index h of 55), and co-guest editor of a RSC book on Nanoscale Thermometry (Nanoscience & Nanotechnology series) and special issues of the Journal of Sol-Gel Science and Technology (2010) and of the Journal of Luminescence (2015). He is editor of Physica B – Condensed Matter, associate editor of the Journal of Luminescence and member of the editorial board of the Journal of Coordination Chemistry, Journal of Sol-Gel Science and Technology and Journal of Rare Earths.

PL16 Fourier transform infrared spectroscopy (FTIR) and Raman spectroscopy

Fourier transform infrared spectroscopy (FTIR) and Raman spectroscopy

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Department of Chemistry
School of Life and Environmental Sciences
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This module will cover several aspects of infrared and Raman spectroscopy that are critical for the materials chemist doing structural and/or compositional characterization. Various chosen spectral examples will be presented and interpreted. Emphasis will be also given to Two-Dimensional Correlation Spectroscopy as a powerful tool to unravel complex spectral bands.

Short CV

Verónica de Zea Bermudez, born in 1962, graduated in Chemical Engineering in 1980 from the Instituto Superior Técnico in Lisbon. She received her MSc. degree in *Chemistry of the Catalytic Processes* from the Instituto Superior Técnico in 1985 and her PhD. degree in *Electrochemistry* from the Institut Polytechnique de Grenoble (France) in 1992.

In 1993 she joined the University of Trás-os-Montes e Alto Douro as Assistant Professor where she assumed responsibility for the Chair of *Materials Science* in the Department of Chemistry. She received her *Aggregation* in *Materials Chemistry* in 2008 and became Full Professor in June 2012. She has been Principal Investigator of the Materials Chemistry Research Group of the Chemistry Center of Vila Real since 2003.

Since 1993 her scientific activity has evolved through the synthesis and characterization of sol-gel derived organic/inorganic hybrids with applications in the domains of solid state electrochemistry (essentially electrochromic devices and fuel cells) and optics. In recent years she has been particularly interested in the development of complex hierarchically structured ordered hybrid materials derived prepared through the combination of sol-gel chemistry reactions and self-assembly routes from commercial or click chemistry-derived organosilanes. Current interests are also focused on the bio-inspired deposition of biominerals on biopolymers and biohybrids for biomedical applications.

She co-authored a U.S. patent in 1994. She published 8 book chapters and more than 160 articles in international journals indexed in the SCI (h-index of 33 and 3637 citations (excluding self-citations).

Short Courses

C1 Scanning electron microscopy (SEM) & Transmission electron microscopy (TEM)

Pedro Tavares
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Augusto Lopes
Departamento de Engenharia de Materiais e Cerâmica
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Please see pages 13 and 14 for the short CVs of the lecturers.

C2 Mechanical essays

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Please see page 15 for the short CV of the lecturer.

C3 X-ray photoelectron spectroscopy (XPS)

Gonzalo Guillermo Otero Irurueta
Professor Auxiliar convidado do Departamento de Engenharia Mecânica
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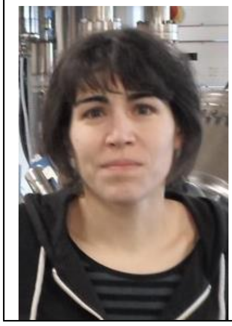

Maria J. Hortigüela
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Short CVs

Gonzalo Otero-Irurueta obtained his PhD in Physics at the Autonomous University of Madrid (Spain) in 2010. During his PhD he studied the surface catalysed cyclodehydrogenation of large polycyclic aromatic hydrocarbons under the supervision of Prof. José Angel Martin-Gago. In 2013 he joined TEMA at Aveiro University as FCT postdoctoral fellow and since 2016 he has the “investigador auxiliar” position.

María J. Hortigüela received his Ph.D. in chemistry from the University of Burgos (Spain, 2009) for a work related to MWCNTs 3D scaffolds developed at the Group of Bioinspired Materials (ICMM, CSIC). She later joined the Recombinant Protein Production Group at NUI Galway as IRSCET postdoctoral fellow. Currently she works at TEMA, University of Aveiro, operating the XPS system.

C4 Differential thermal analysis (DTA), Thermogravimetry (TGA) and differential scanning calorimetry (DSC)

José António Morais Catita
Director Técnico na Paralab
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The course will be conducted based on the sample preparation and interpretation of different results. The following topics will be addressed.

-Types of Thermal Analysis

-Sample preparation

-Method design according to different purposes

-Critical variables for the analysis.

-Typical curve shapes for typical phenomena

-Measurement procedure

-Results interpretation and Validation

Short CV

Born in 1969, he is a PharmD with a PhD in Analytical Chemistry both from the University of Oporto.

Recently, he concluded a post-graduation in Management and Business Administration from the Catholic University Business School.

Professor at the Faculty of Health Sciences – UFP, teaching in the fields of Biophysics, Physical-Chemistry and Advanced Analytical Techniques. He is author or co-author of several peer reviewed publications, oral presentations and invited lectures. His main interests are related to materials characterization, namely for their physical properties.

In parallel, he is Senior Manager and Technical Director at PARALAB SA (Portugal) and PARALAB SL (Spain).

He acts regularly as technical consultant for the development and validation of analytical methods in highly regulated industries, namely pharmaceutical industry.

Since 2011, he is an Independent Expert Evaluator at the European Commission and has been involved in the evaluation of several projects related with nanomaterials characterization.

C5 Filmes de Langmuir/Langmuir-Blodgett, Balança de Langmuir e caracterização (BAM, AFM, RX)

Eduardo Jorge Morilla Filipe
Departamento de Engenharia Química e Biológica
Instituto Superior Técnico
Universidade Técnica de Lisboa
Av. Rovisco Pais, 1049-001 Lisboa, Portugal
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Please see page 26 for the short CV of the lecturer.

C6 Atomic force microscopy (AFM)

Andrei Kholkin
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Please see page 23 for the short CV of the lecturer.

C7 X-ray diffraction (XRD)

José António de Carvalho Paixão
Universidade de Coimbra
Faculdade de Ciências e Tecnologia
Departamento de Física
Rua Larga P-3004-516 Coimbra Portugal
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A hands-on course on PXRD, covering sample preparation, data-collection and analysis (phase identification and quantification, Rietveld refinement).

Please see page 29 for a short CV of Professor José A. C. Paixão.

C8 Rheology

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Rheology is now well established as the science of the deformation and flow of matter. It is the study of the manner in which materials respond to applied stress or strain. All materials have rheological properties and the area is relevant in many fields of study as polymers and composites, plastics processing, cosmetics, food, bioengineering, structural materials, among others.

This presentation will introduce participants to rheology fundamentals (viscosity profiling, thixotropy, viscoelastic properties), principles of measurements and sample characterization procedures.

Short CV

Pedro Miguel Prazeres graduate in Industrial Chemistry at University of Coimbra in 2006 where he has developed some research work on mutual diffusion coefficients using Taylor Dispersion Technique resulting in 2 co-authored publications. Since 2007 he has been working with rotational rheometers as product manager / product specialist being responsible for users training and applications support.

C9 Dynamic light scattering (DLS)

José António Morais Catita
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The course will be conducted in an interactive mode with the participation of the attendees. It will start with some simple analysis and from there the following topics will be addressed.

-The phenomenon of light Scattering

-Terms and definitions

-Normative references

-Principle of DLS

-DLS optical detection – The Correlogram

-Calculation of mean particle size and PdI – The Cummulants analysis

-Intensity Distribution – The NNLS model

-Figures of Merit

-Test sample preparation

-Measurement procedure

-Results interpretation and Validation

Please see page 35 for a short CV of José Catita.

C10 Solid-State Nuclear Magnetic Resonance (SSNMR)

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Maria João Ferreira
Centro de Química Estrutural
Instituto Superior Técnico
Universidade de Lisboa
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Short CVs

Mariana Sardo got her degree in Physics and Chemistry for teaching in 2005 (University of Aveiro) followed by a PhD in Raman Spectroscopy (completed in 2009, University of Aveiro), studying weak intermolecular interactions in functional materials, pharmaceutics and inclusion compounds. For the post-doctoral research, solid-state NMR was the topic of choice. After an initial 1-year period in the group of Prof. Beat Meier at ETH-Zurich, performing structural studies of proteins, her work continued in the group of Prof. João Rocha and Dr. Luís Mafra, employing high-resolution solid-state NMR spectroscopy at high magic-angle spinning frequencies for structural and dynamic studies of small molecules, pharmaceuticals and encapsulated compounds. Characterization and atomic-level understanding of different types of materials (zeolites, ceramic glasses, MOFs, PMOs, ZIFs, etc.), surface interactions and host-guest interactions has also been a major component of her most recent research work.

M.J. Ferreira (MJF) graduated in Chemical Engineering, with specialization in Applied Chemistry, from IST in 1998. She worked in the Laboratory of Organometallic Chemistry (IST) as a Research Assistant (1999-2001) and as a PhD student (2001- 2006) with Prof. A.M. Martins where she synthesized and studied the reactivity of Ti and Zr complexes. In 2006 she moved to Vancouver, Canada, where she worked as a postdoc with Prof. M.D. Fryzuk (UBC) in N2 activation and functionalization. In 2008 she moved to Heidelberg (Germany) to work as a postdoc with Prof. P. Hofmann at CaRLa–Catalysis Research Laboratory, a laboratory incorporated at the U. Heidelberg and supported by BASF. She studied C-H activation coupled to amination with Pt and Pd complexes and collaborated with Dr. M. Limbach (BASF) and Prof. Hashmi (U. Heidelberg) in gold chemistry and catalysis. In addition, she was responsible for CaRLa's NMR facility. In 2011 moved to Brazil where she worked as postdoc at UFMG, Belo Horizonte, under the supervision of Prof. E.N.dos Santos in olefin metathesis. In 2012 she moved back to Portugal to work with Dr. P. Ferreira and Dr. L. Mafra (U. Aveiro) on a project involving imidazolium based materials for CO_2 capture and conversion. She is currently working at IST in Applied NMR, with Profs. J. Ascenso and T. Nunes and is currently responsible for maintaining 4 NMR spectrometers (solid and liquid state).

C11 Porosimetry, adsorption (BET)

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This course will cover two different techniques, BET and Mercury Porosimetry, that together, are able to characterize the porous structure of materials from 4 A up to almost 1 mm (micro, meso and macropores).

BET - It will be presented the basic principles behind the technique, how it works, and all major methods to process data and get porous size information.

Mercury Porosimetry – it will be discussed the basic principles behind this technique, how it works and how to process measured data to get not only pore size distributions but also other parameters like porosity, diffusion, compressibility, particle average size, and others.

Short CV

In 1990 Rui Soares got the degree in Chemical Engineering at the Engineering School of Porto University. From 1990 to 1994, also on the same department, he was involved in research projects related to catalysis, reaction engineering and automation of experimental setups. He was co-author of chapters on three books, one paper and made several oral presentations on international congresses.

Founding member of PARALAB, he is since 1994 its CEO. Since 2012 he is accumulating the position of CEO of PARALAB SL (Spain). The Paralab's business segment on 'Development of New Products' where automated experimental setups are developed to customer's requirements, is also lead by Rui Soares.

He is the PARALAB's Product Specialist for Porous Materials Characterization and GPC (Gel Permeation Chromatography).

C12 Contact angle

João Carvalheira
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Paralab

Contact Angle Measurement by optical tensiometry is an extremely versatile technique used to characterize material properties related to wettability, adhesion and homogeneity. It is used to characterize material surface properties and interfacial interactions between gas, liquid and solid phases. Optical tensiometers are used in R&D and quality control in a variety of industries, including biomaterials, chemicals, pharmaceuticals, electronics, foods, energy, environment, paper and packaging.

This course will be conducted in an interactive mode with the participation of the attendees. It will be show how Contact Angle measurements can be used for surface characterization. Properties as Surface Tension, Surface Energy, Work of Adhesion, Wettability and Roughness will be presented and measured by a Contact Angle Meter with Topography module.

Short CV

João Sarmento Carvalheira graduated in Chemical Engineering at the University of Porto in 2000. In 2016 he concluded a post-graduation in Marketing Management at the Católica Porto Business School. Since 2012 he is Product Manager at Paralab for Material Characterization instrumentation. He has been working with Contact Angle Meters since 2001, being responsible for its marketing, installation and training.

C13 Thermal conductivity and infrared thermography

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The Laboratory Session C13 will demonstrate the use of techniques available at UA:

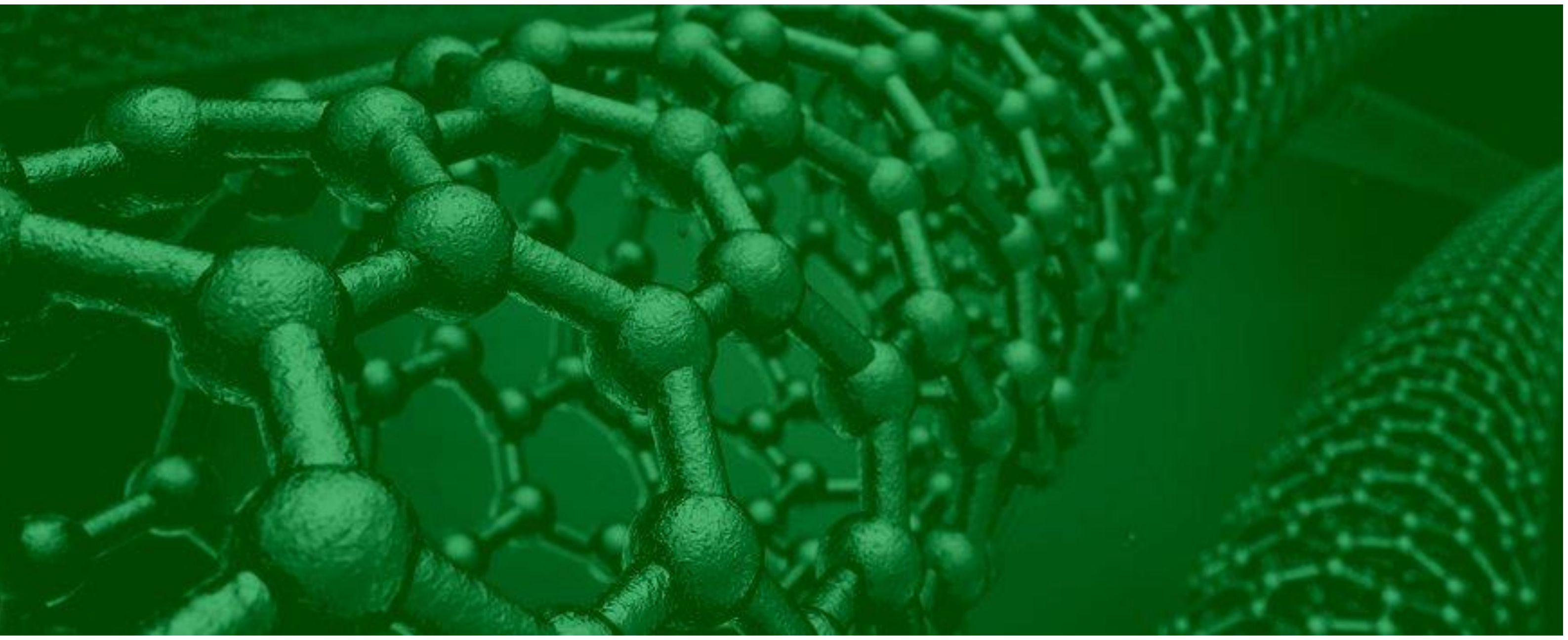
1) For thermal conductivity (and specific heat), the Gustafsson Probe (Hot Disk, Transient Plane Source TPS 2500S) method allowing the accurate measurement of both liquids and solids (bulk or porous) with conductivities ranging from 0.005 to 1800 W/m/K, in a broad temperature range, with bath (-20ºC to 180ºC) and oven (up to 750ºC). Its applications in solid materials spans from highly insulating aerogels and foams, polymers, ceramics to conducting metals and liquids like milk or carbon nanotube filled refrigerants. It can also handle thin films/coatings, and thermal conductivity anisotropy.

2) For thermal imaging, a FLIR 5600 Infrared thermography camera with microscope accessory will be demonstrated, allowing acquisition times down to 1 ms, sensitivity ~ 20 mK, and spatial resolution ~5 micrometers, convenient for the study of fast processes and small temperature gradients. The thermal mapping also allows the direct measurement of thermal diffusivity and its anisotropy in materials with the technique of thermal ellipsometry.

3) Combined with AFM microscope, Scanning Thermal Microscopy (SThM), in our XE7 Scanning Probe Microscope, Park Systems allows mapping thermal conductivity at the nano-scale (~50 nm) resolution and using heater/thermometer tips also can be used to perform thermal analysis and phase transition detection, mapping inhomogeneities, on coatings and composite materials.

The Laboratory Installation was financed by project Heat@UA "Facing the challenges of characterizing novel thermal materials and processes" RECI/CTM-CER/0336/2012 with team members of two Associated laboratories (CICECO and I3N) and two Research Units (TEMA and RISCO).

Please see page 31 for the short CV of Professor Vitor Amaral.



Poster Presentations

GROWTH OF FUNCTIONAL PROTEIN FIBRILS FROM EGG WHITE PROTEOME: EFFECT OF PROTEIN CROWDING

Pankaj Bharmoria,[1] Dibyendu Mondal,[1*] Matheus M. Pereira,[1]
Márcia C. Neves,[1] Mafalda R. Almeida,[1] Igor Bdikin,[2]
João A. P. Coutinho,[1] Mara G. Freire[1]

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Keywords: Protein fibrils; Ionic liquids; Egg white proteome

In recent years, protein fibrils have attracted a large attention as advanced functional biomaterials for biotechnological applications [1]. However, their large scale application is limited by some drawbacks, such as a poor scalability, slow synthesis kinetics and high cost [2]. In the present work, we had overcome these limitations and herein report a fast and bulk scale fibrillation of proteins from egg white proteome (EWP) using ionic liquids (ILs) as fibrillating agents. The rapid fibrillation is governed by the effect of protein crowding, with enhanced protein-protein interactions upon intercalation with ILs. Instant fibrillation of EWP upon addition of ILs was observed from microscopic analysis and further confirmed from TEM and AFM imaging. The fluorescence changes of thioflavin T dye upon binding to protein fibrils confirmed the fast growth of protein fibrils [3]. UV-Vis and FT-IR were used to address the structural changes in EWP upon fibrillation. The effect of protein crowding on fibrillation (protein-protein and protein-IL interactions) was analysed by molecular docking. The prepared fibrils are also a biocompatible support for enzymes, as observed with cytochrome c, in which a 2.5-fold increase in activity was observed. A larger scale study further confirmed that 100 g of protein fibrils can be produced from 1L of EWP though a cost effective and greener process. With the approach here proposed, the problems of long time production process, scalability and high cost associated to protein fibrils are overcame.

References

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Acknowledgements

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P2

FORMATION OF POLY(LACTIDE) STEREOCOMPLEXES IN BLENDS WITH A CHOLINIUM IONIC LIQUID

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Keywords: Polylactic acid, stereocomplex, ionic liquids.

Biodegradable polymers bring a significant contribution to the sustainable development in view of the available attractive methods for disposal with minor environmental impact. Aliphatic polyesters represent a large part of biodegradable polymers and among these, poly(lactic acid) (PLA) appear to be one of the most attractive because of its availability and biodegradability [1]. PLA has extensive applications in packaging, biomedical fields, including suture, bone fixation material, drug delivery microsphere, and tissue engineering [2]. A great variety of techniques and additives have been evaluated to improve the physicochemical properties of PLA and enlarge its range of application [3].

In this study we report a novel method to produce poly(lactic acid) (PLA) stereocomplex (SC) crystallites from high molecular weight PLA by incorporation of choline dihydrogen phosphate ([Ch][DHP]) ionic liquid into the PLA matrix at room temperature. The morphology of membranes with 5% wt. and 10% wt. [Ch][DHP] consists of PLA microspheres with enhanced crystallinity and ca. 50-60 μm in diameter, which are formed due to the PLA/ [Ch][DHP] immiscibility. The electrical conductivity of these membranes measured by impedance spectroscopy is in the range $6x10^{-7}$–$4x10^{-6}$ Scm^{-1} increasing with the content of choline and with increasing relative humidity (RH). Combined results of X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and differential scanning calorimetry (DSC) confirm the formation of the PLA SC crystals. On the other hand, piezoresponse force microscopy (PFM) and atomic force microscopy (AFM) revealed a new phase with enhanced piezoelectric properties at the microsphere interfaces, which is directly related with the formation of SC crystalline domains. These novel biomembranes provide a novel, cost-effective and faster synthetic method to produce PLA SC and reinforcing the potential of this new morphology to produce soft piezoelectric mats.

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Acknowledgements

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PURIFICATION OF IMMUNOGLOBULIN Y (IGY) USING MODIFIED MAGNETIC IRON OXIDE NANOPARTICLES

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Due to the actual emergence of antibiotic-resistant pathogens, the application of antigen-specific antibodies in passive immunotherapy represents an imperative reality in the near future. In addition to the more investigated mammal antibodies, antibodies from egg yolk (IgY) can be obtained in higher titres and by non-invasive methodologies [1]. Up to date, several methods, such as precipitation, dialysis, ultrafiltration and chromatography are available for IgY purification [2]. Nevertheless, the production cost of IgY still remains higher than other drug therapies due to the lack of cost-effective purification techniques. The development of a cost-effective and scalable new strategy for the purification of IgY is thus in high demand and will have a high impact in economics and human health. In this work, a new platform for the purification of IgY using functionalized magnetic nanoparticles (FMN) was investigated. Magnetic nanoparticles (Fe_3O_4) were synthesized, coated with silica and functionalized [3], and also characterized in terms of their morphological, chemical and structural features. The immunoglobulin extraction assays with magnetic particles were carried out envisaging the development of a new method of purification, and where extraction yields up to 93% and purification levels up to 94% have been obtained.

References

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Acknowledgements

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P4

SYNTHESIS AND CHARACTERIZATION OF CRYPTOMELANE-TYPE MANGANESE OXIDE CATALYST FOR VOC CONTROL

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Keywords: Cryptomelane; Manganese oxides; Volatile organic compounds

The emission of volatile organic compounds (VOCs) entails several environmental and human health problems. Catalytic oxidation is one of the most efficient and economically viable technologies for VOC removal. Cryptomelane-type manganese oxides have already shown high activity for the oxidation of several VOCs, normally ascribed to the mixed valence of manganese and mobility of the lattice oxygen. Cryptomelane is an octahedral molecular sieve composed of 2 x 2 edge and corner shared MnO_6 chains forming a tunnel structure with potassium ions present inside the structure. In this work, cryptomelane-type manganese oxides were prepared by a novel solvent-free method, using a ball mill to mix potassium permanganate and manganese acetate. The mixture is then kept at 80 ºC for 4 h, washed with distilled water, dried at 100 ºC and finally calcined at 450 ºC for 4.5 h.

The produced material was characterized by several techniques. N_2 adsorption isotherm at -196 ºC was performed in order to calculate the BET surface area (S_{BET}). The isotherms of the material were of type IV according to IUPAC classification, which are characteristic of mesoporous materials. The material has a S_{BET} of 120 $m^2 g^{-1}$, which is significantly higher than that of cryptomelane produced by the conventional reflux method [1]. X-ray diffraction (XRD) analysis showed that the material was pure cryptomelane. Photoelectron spectroscopy (XPS) analysis was performed in order to evaluate the surface oxygen and the average oxidation state (AOS). The O 1s spectrum showed that lattice oxygen is the most abundant oxygen specie in the cryptomelane surface (75 wt%). Lattice oxygen is considered to play a key role in the catalytic oxidation of VOCs. The AOS was calculated using the Mn 3s region. The value obtained was 3.68, showing the mixed valence state of manganese, which is known to be beneficial to the oxidation reaction.

The catalytic activity of the material was evaluated in the oxidation of ethyl acetate (ester), ethanol (alcohol) and toluene (aromatic hydrocarbon). The cryptomelane catalyst presented a high catalytic activity for the conversion of ethyl acetate and ethanol into CO_2, achieving 90 % conversion at 203 and 201 ºC, respectively, but a much lower for toluene conversion, with 270 ºC being required to obtain 90 % conversion into CO_2.

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LUMINESCENT ELECTROCHROMIC DEVICES INCORPORATING ORGANIC/INORGANIC (BIO)HYBRID ELECTROLYTES

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Keywords: Lanthanides, (bio)hybrid electrolytes, electrochromic devices

The increasing energy request in the world as led to a global dependence on fossil fuels to supply these needs. As a consequence, the CO_2 levels are growing dramatically and the corresponding climate changes can be catastrophic. Because the building sector is a major energy consumer and represents about 40% of the total energy consumption in the European Union, where a very significant amount of that energy is used for heating and cooling, one action that will save energy is increasing the energy efficiency of buildings [1,2]. Fenestration products play an important role in energy saving, since up to 60% of the total energy loss of a building comes from its windows [3].

Electrochromic devices (ECDs) have emerged as a “green” technology and have a high potential when applied to windows (smart windows) by changing properties, such as the solar factor and the visible transmission of radiation of the solar spectrum in response to an electric voltage. This allows to reduce the request for electric lighting, and cooling and heating loads resulting in a drastic decrease of energy consumption in glazed-buildings [3]. This is particularly important in Northern and Eastern European countries and North America. In cold climate regions, smart windows with uninterrupted near-infrared (NIR) light transmission are the ultimate request for energy-efficient buildings.

Organically modified silicate electrolytes (ormolytes) have been used to produce ECDs since the sol–gel process is one of the preferred methods to fabricate these devices. Ormolytes are extremely attractive given their unique characteristics (typically amorphous, highly transparent, and homogenous). In the sol state, they may be easily deposited to form thin films via non-traditional, simple and cheap coating techniques, such as spin-coating. The resulting xerogels exhibit appropriate mechanical, chemical and thermal stability, and can accommodate large amounts of guest salts [4]. In the present work, luminescent ECDs based on ormolytes composed by a room temperature white light emitting hybrid host structure doped with lanthanide ions (e.g., Eu^{3+} and Er^{3+}) will be produced and characterized featuring applications in luminescent ECDs.

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P6

TOWARDS PHOSPHONIC ACID PORPHYRIN-BASED NANO-METAL-ORGANIC FRAMEWORKS

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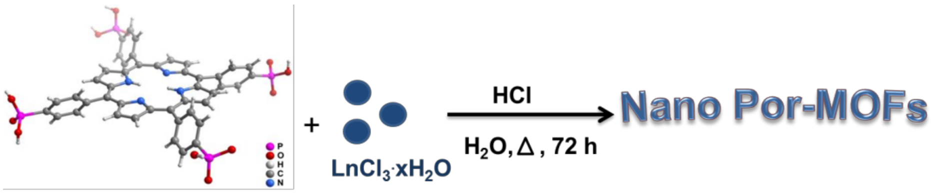
Keywords: porphyrin, phosphonic acids, metal-organic frameworks

Metal-Organic Frameworks (MOFs) constitute an outstanding class of crystalline and porous materials that has known a great surge in recent years [1]. These materials are prepared from metal ions, or cluster nodes, and organic linkers and because of the endless number of potential combinations between these units, it is easy to recognize the huge diversity regarding their structural diversity. Porphyrins (Pors) arise as peculiar construction building units which give rise to a fascinating niche of MOFs – Porphyrin-based MOFs (Por-MOFs) [2]. Por-MOFs have already demonstrated their potential as promising materials for a variety of applications including, but not limited to catalysis [3], gas separation and storage, as well as light harvesting [4].

Herein, we report the preparation of unprecedented phosphonic acid Porphyrin-based Nano-Metal-Organic Frameworks, and their strucural characterization using varioustechniques: powder X-ray diffraction (PXRD), scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDS), ultraviolet-visible (UV-Vis), scanning transmission electron microscopy (STEM), dynamic light scattering (DLS), solid-state NMR and Fourier transform-infrared spectroscopy (FT-IR). The thermal robustness was also evaluated using thermogravimetry and thermodifractometry.



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SCREENING THE PREPARATION OF NEW FUNCTIONAL BIO-MOFs WITH ADVANCED CHARACTERIZATION TECHNIQUES

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Keywords: Metal-Organic Frameworks; Advanced Characterization Techniques

Metal-Organic Frameworks (MOFs) are a class of materials of growing interest. MOFs allow combining different metal ions and organic linkers into coordination-based networks to provide a wide variety of materials with applications in the most diverse areas. Concerning bio-applications, research has been driven by the ability of MOFs to deliver large quantities of drugs, along with their capacity to combine the therapeutic properties of different substances used as part of the network itself.

The present work deals with alendronate-calcium MOFs and their characterization, in which several techniques play a key role. Powder X-Ray Diffraction (PXRD) allows the identification of new alendronate-calcium bio-MOF materials through the identification of new crystalline phases. Also, this technique gives information about the purity of the obtained MOFs, which is of extremely high relevance for the following steps concerning their application. Along with PXRD, ^{31}P Nuclear Magnetic Resonance (NMR) also provides important information about the purity of the synthesized bio-MOF. Furthermore, Thermogravimetry (TGA) and Scanning Electron Microscopy (SEM) analyses provide data on the thermal behavior and particle morphology of the new bio-MOFs, respectively. Taken together, results from these techniques help to identify new bio-MOFs composed by alendronate and calcium and, at the same time, provide information about their properties, making ground for future bio-applications.

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P8

AN INVITATION TO MAGNETISM

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Keywords: magnetism, SQUID

Magnetic properties and phenomena encompass a very large range of scales, from sub-atomic particles to large scale objects. In modern experimental studies for magnetic materials development, high resolution properties characterization are crucial to understand the behavior of thin films, heterostructures or nanoparticles, and assess their performance for device or bio-medical applications. On the other hand, molecular and low dimensional system magnets are a challenging field for new and versatile multifunctional applications.

The installation in 2015 of the new Quantum Design MPMS3 SQUID-VSM Magnetometer brought the capability of performing studies in the temperature range from 1.8K up to 400K and magnetic fields up to 7 Tesla, with noise level below 10^{-8} e.m.u (equivalent to 10^{-10} g or 20 $(\mu m)^3$ of magnetite). The cryogenic system allows fast and stable studies of small, weak signal samples.

This poster presentation reports in general some of the recent work, emphasizing demanding situations, which in some cases require the use of more complex data analysis and modelling to account for finer details (and impurities) detected.

Its aim is to give an overview of capabilities and invite to add some magnetic spice to your research.

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P9

METAL-ORGANIC FRAMEWORK BASED ON HIGHLY FLEXIBLE TETRAPODAL ORGANIC LINKER

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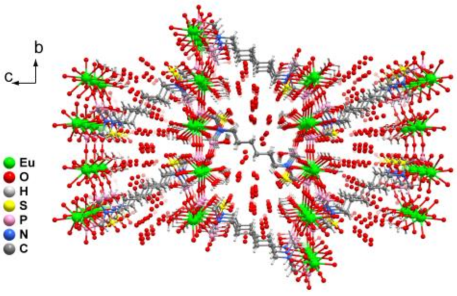
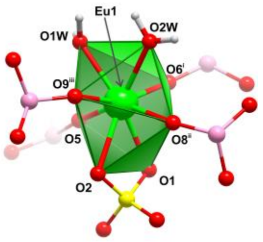
Keywords: Metal-Organic Framework; solid-state characterization

Metal-Organic Frameworks (MOFs) and Coordination Polymers (CPs) are highly ordered crystalline compounds based on the self-assembly of metal centers with a myriad of organic linkers. By taking into consideration the high versatility of these networks [1,2] this research area is currently driven by the need to employ these materials in important technological areas for society.

In this work, a new Metal-Organic Framework based on a highly flexible tetraphosphonic acid organic linker, hexamethylenediamine-*N,N,N',N'*-tetrakis(methylphosphonic acid) (H_8htp), is reported. $[Eu_2(SO_4)_2(H_6htp)(H_2O)_4]\cdot 10H_2O$ (**1**) was obtained by microwave heating at moderate temperatures (80 ºC) and low reaction times (15 minutes). The reaction is carried out in aqueous medium and because of the high flexibility of the organic linker sulfuric acid was added in small quantities. When compared to the uniquely reported material based on the same building blocks, this synthetic approach allowed us to significantly reduce the reaction time to just 15 min with an immediate crystal formation (compared to the 2 months reported in the literature). Crystals were obtained with sizes suitable for single-crystal X-ray diffraction studies.The material consistsof a compact 3D network with the metal centers forming a packed layer which, in the crystal structure, is interconnected by the organic linker. This leads to a high number of cavities which are filled with water molecules. The MOF was further characterized using several solid-state techniques, such as FT-IR, solid-state NMR and thermogravimetry.





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P10

CARBON NANOTUBE-BASED HETEROSTRUCTURES INVESTIGATED BY ANALYTICAL TRANSMISSION ELECTRON MICROSCOPY

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Keywords: Atomic layer deposition, metal oxides, carbon nanotubes

The controlled deposition of thin films on high surface area supports are prerequisites for a rational design of interfaces and the production of multifunctional materials. Atomic layer deposition (ALD) emerges as a powerful and versatile technique for the coating or decoration of high surface area supports. It permits a precise deposition of conformal and homogenous thin films, based on a reaction between precursor materials, which are separated into successive surface reactions. Accordingly, the reactants are kept separated reacting with surface species in a self-limiting process, i.e. without the presence of gas phase reactions. The conformal growth of the ALD film is a direct consequence of self-limited surface reaction and the film thickness is determined by the number of cycles. ALD technique is widely used for metal oxide thin films deposition, which formation involves the reaction between a metal precursor and an oxygen source [1,2]. ALD is, therefore, specifically suited for the elaboration of heterostructures. In the present work, it is highlighted the versatility of ALD approach for the precise coating of nitrogen doped- and pure-carbon nanotubes. The process was successfully applied for thin films of metal oxides (e.g. Mn_3O_4 or ZnO), preserving the support geometry. The obtained heterostructures are definitely, suitable for a variety of applications in different fields such as microelectronics, energy conversion and chemical catalysis.

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P11

SUGAR DERIVED CARBON SPHERES AS ESTERIFICATION CATALYSTS

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Keywords: Hydrochar; Hydrothermal; Carbon Spheres: Esterification

Carbon spheres have been used in different research fields, namely as supercapacitors, adsorbents, catalyst supports, and also as catalysts. [1] The most common synthesis strategy involves hydrothermal treatments, and as carbon precursors, although various renewable biomasses have been explored, a great number of studies are based on sugar derived materials. [2]

In the studies that are being developed, glucose, fructose and sucrose derived carbon spheres obtained by hydrothermal treatment at 190 ºC were tested as catalysts for the esterification of acetic acid with 1-butanol. The materials have acidic surface properties, demonstrated by the presence of carboxylic acids and alcohols, estimated by the Bohem titration, and pH_{pzc} values (*ca*. 2.0). Besides the as synthesized materials also samples treated with concentrated H_2SO_4 were assayed. The introduction of sulfonic groups has a positive effect on the reaction yield which in the more favorable case reaches 95 % after 6 h of reaction. The results obtained so far point out the potentialities of these materials as alternatives to the commonly used strong inorganic acids.

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P12

MAGNETIC NANOPARTICLES AS PLATFORM FOR THE ELECTROCHEMICALGENOSENSING OF GENETICALLY MODIFIED SOYBEAN

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Keywords: Core-shell Fe_3O_4@Au magnetic nanoparticles, genoassay, genetically modified soybean

Nowadays, there is a growing interest on the development of high throughput tools able to rapidly assess the presence of genetically modified organisms (GMO) in food and feed products. In the case of complex samples, magnetic separation is one of the easiest ways to separate the component of interest from the rest of the constituents of the sample. Core-shell gold-coated iron oxide magnetic nanoparticles (Fe_xO_y@Au MNPs) have been attracting considerable interest in the bioassays field owing to their superparamagnetic properties and easy functionalization of the gold shell with thiolated molecules leading to the formation of a self-assembled monolayer (SAM), which allows obtaining a well-defined and organized surface, long-term stability and biocompatibility [1].

In this work, monodisperse Fe_3O_4 MNPs were synthesized by thermal decomposition and subsequently coated with a gold shell through reduction of $HAuCl_4$ on the surface of the MNPs in the presence of an organic capping agent. Two SAMs were studied in order to understand the effect of the presence / absence of the blocking agent (6-mercapto-1hexanol) on the surface of MNPs and how the electrochemical signal is affected. The samples were characterized by transmission electron microscopy (TEM), energy dispersive X-ray spectroscopy (EDX), UV-VIS spectroscopy, Fourier transform infrared spectroscopy (FTIR) and Raman spectroscopy with the objective of studying the morphology, particle size and chemical composition.

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PRIMARY LUMINESCENT THERMOMETERS OPERATING IN DIFFERENT MEDIA BASED ON SILICON NANOPARTICLES

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Keywords: luminescent thermometry, primary and self-calibrated thermometer, hyperspectral microscopy

Luminescent thermometers operating at the nanoscale, where the conventional methods are ineffective, have emerged as a very active field of research. Luminescent crystalline silicon nanoparticles (SiNPs) are a promising choice for nanothermometry, combining the Si biocompatibility with the potential compatibility with the current microelectronic technology [1]. The thermal dependence of the emission peak position of SiNPs is well-described by the Varshni's law, enabling the development of a self-calibrated nanothermometer with a calibration curve predicted by a such well-stablished state equation and avoiding new calibration procedures whenever the thermometer operates in different media [2].

In this work, SiNPs functionalized with 1-dodecene were used to produce film- and solution-based luminescent nanothermometers. In the case of film's, we show from measurements with a hyperspectral camera (pixel field-of-view of 1.3×1.3 μm^2) that the emission is homogenous across the surface, at least at the microscale. We demonstrate, for the first time, that luminescent thermometers based on SiNPs films and solutions, with the thermometric parameter predicted by a well-established equation, enable temperature sensing independent of the medium (air, vacuum, nitrogen atmosphere). The nanothermometer calibration curve is predicted by Varshni's law and allows temperature sensing in a wide range of temperatures from cryogenic to 480 K, with maximum relative sensitivity of 0.04 $\%.K^{-1}$ and reversibility and repeatability above 99.98 %.

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P14

DEVELOPMENT OF A NEW PLATAFFORM FOR IgY PURIFICATION USING CARBON BASED NANOMATERIALS

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Keywords: Immunoglobulin Y, Carbon xerogels, Purification

Due to the current rise of drug-resistant microorganisms, passive immunization employing antibodies has become a hot topic of research [1]. In this context, an emerging alternative consists in the investigation of antibodies existent in egg yolk (immunoglobulin Y, IgY), which play a similar biological role as traditional mammal antibodies (IgG). The use of IgY offers advantages such as high availability (50-100 mg IgY per egg) and the reduction of painful manipulations, e.g. the stressful cruel bleeding of animals to obtain the serum [2]. In fact, chicken IgY can be easily obtained by a non-invasive collection of eggs. Classical approaches have shown to be time-consuming and not able to provide high IgY purification factors [2]. The use of nanostructured carbon materials, such as carbon xerogels (CX), appears as a new promising alternative for the extraction and purification of IgY.

The present work focuses on the extraction and purification of IgY from egg yolk using CX materials with controlled porosity (pore diameters of 3, 4, 13 and 30 nm). The extraction of IgY was based on the adsorption of smaller and contaminant proteins present in the water soluble protein fraction (WSPF) obtained from egg yolk promoted by the contact between the nanomaterial and the WSPF. The most promising materials are those with a porosity of 3 nm and 13 nm, with a purification level of IgY above 50% in both cases, and an IgY recovery yield above 50% and 89%, respectively. CX materials represent a new approach to purify IgY while envisaging their use as alternative biopharmaceuticals in the near future.

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ESTABLISHMENT OF A DATABASE FOR FORENSIC DISCRIMINATION OF LATEX GLOVES

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Keywords: latex gloves, polyisoprene, forensic chemistry

Latex gloves are frequently used by felons to avoid leaving fingerprints and DNA proves in crime scenes. The majority of felons discard the gloves at the crime scene or nearby [1-3]. Despite being common items, an extensive analysis of latex gloves may provide useful information to crime scene investigators. In fact, in some cases, it may be useful to compare gloves found at the crime scene with those seized at the suspect's premises or in context of smuggle illegal drugs in *body stuffers* [3].

Latex is a highly regular *cis*-1,4-polyisoprene produced by more than 2000 species. The manufacture of latex gloves involves a compounding step, which allows to improve their final properties [1]. This step and the differences along the general manufacture process enable distinguishing glove origins from one another.

The main objective of this study is the development of a database for discrimination of latex gloves that are indistinguishable by visual examination, using a multidisciplinary approach, without any sample preparation, combining infrared spectroscopy in attenuated total reflectance mode (FTIR-ATR), differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), polarized light microscopy (PLM) and X-ray diffraction (XRD).

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P16

EFFECT OF GRAPE POMACE EXTRACTS ON CHITOSAN FILMS PHYSICOCHEMICAL PROPERTIES

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Keywords: Atomic force microscopy; Mechanical properties; Antioxidant activity

The use of edible films and coatings in food protection and preservation from renewable biopolymers has recently increased due to its nontoxicity, biocompatibility, and antimicrobial properties. Further, edible films can be an efficient vehicle for incorporating functional compounds, which improve its characteristics. Grape pomace consisting of skins, seeds, and stems, is a rich source of phenolic compounds, lipids, polysaccharides and proteins. Since grape pomace is an abundant by-product, there is a high interest to use its extracts in order to improve the chitosan films properties.

This work consists in the preparation of chitosan-based films with improved properties for food applications. Three grape pomace fractions are incorporated: 1) hot water extract, with 72 % polysaccharides; 2) chloroform extract, rich in waxes; and 3) n-hexane extract, with the oil, comprising 70 % linoleic acid. As control, a film only with chitosan is also prepared.

The chitosan-based films were homogenous without cracks or macropores by a macroscopic point of view. However, using AFM, it was possible to verify that all films presented roughness. The chitosan film with the incorporation of the aqueous extract showed a more homogeneous and smoother surface compared with the other films. The incorporation of higher proportion of wax and oil led to changes in mechanical properties of the films, namely lower resistance and stiffness. The chitosan-based films with 0.75% oil demonstrated a 75% decrease of solubility in water, due to their hydrophobicity, as confirmed by the contact angle and surface free energy measurements. The hydrophobic films showed higher antioxidant capacity in organic medium (ABTS and DPPH assays) whereas the most hydrophilic films showed an improvement in FRAP and reducing power assays [1].

The chitosan-based films prepared by incorporation of extracts obtained from grape pomace present different and enhanced properties that can be applied in several food preservation applications.

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P17

OLEFIN OXIDATION USING COBALT AND 5-AMINOISOPHTHALIC ACID COORDINATION POLYMERS

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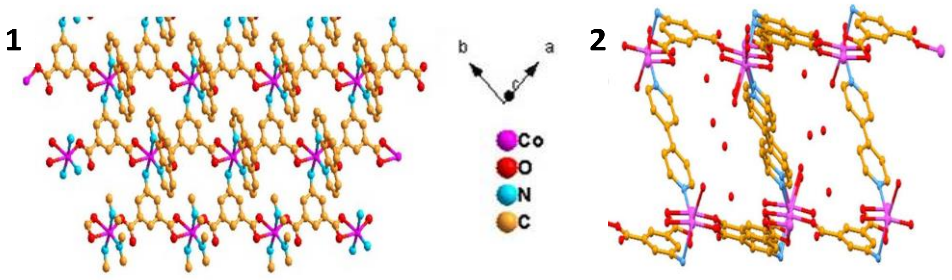
Keywords: Cobalt, Catalysis, PXRD

The demand for new materials that can be used in heterogeneous catalysis is constant. One of those materials are coordination polymers (CPs), which are strongly influenced by their structural features – like the metal coordination environments.[1]

In our group we are using 5-aminoisophthalic acid (H_2aip) to prepare new functional CPs, with luminescent and/or catalytic properties. Two crystalline materials were prepared using hydrothermal and microwave-assisted synthesis and their structures were determined by single-crystal X-ray diffraction (XRD). Both CPs were further characterized by FT-IR spectroscopy, powder XRD, ICP and SEM. The CPs were formulated as [Co(aip)(phen)] (**1**) and $[Co(aip)(bpy)_{1/2}(H_2O)].2H_2O$ (**2**) where phen and bpy correspond to 1,10-phenanthroline and 4,4'-bipyridine, respectively (Figure 1). Both possess 2D extended structures with microporous host frameworks containing 1D channels and the second one (**2**) contains water molecules in some of the channels.

Their application as heterogeneous catalysts in oxidation reactions was studied. *Cis*-cyclooctene and styrene were used as substrates and two different oxidative agents, H_2O_2 (hydrogen peroxide) and TBHP (*tert*-butyl hydroperoxide) were applied. Comparative results between the CPs will be discussed, as well as the characterization of **2** before and after the catalysis.



[Co(aip)(phen)] **$[Co(aip)(bpy)_{1/2}(H_2O)].2H_2O$**

Figure 1. Packing arrangements of coordination polymers **1** and **2**.

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P18

ROBUST MULTIFUNCTIONAL YTTRIUM-BASED METAL-ORGANIC FRAMEWORKS WITH BEATHING EFFECT

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Keyword(s): Metal-Organic Frameworks; Phosphonic acids; Breathing effect

Phosphonate and yttrium-based Metal-Organic Frameworks (MOFs), formulated as $[Y(H_5btp)]\cdot5.5H_2O$ (**1**), $[Y(H_5btp)]\cdot2.5H_2O$ (**2**), $(H_3O)[Y_2(H_5btp)(H_4btp)]\cdot H_2O$ (**3**) and $[Y(H_5btp)]\cdot H_2O\cdot0.5(MeOH)$ (**4**), were prepared using a "green" microwave-assisted synthesis methodology which promoted the self-assembly of the tetraphosphonic organic linker [1,1'-biphenyl]-3,3',5,5'-tetrayltetrakis(phosphonic acid) (H_8btp) with Y^{3+} cations. This new family of functional materials, isolated in bulk quantities, exhibits a remarkable breathing effect. Structural flexibility was thoroughly studied by means of X-ray crystallography, thermogravimetry, variable-temperature X-ray diffraction and dehydration and rehydration processes, ultimately evidencing a remarkable reversible Single-Crystal to Single-Crystal (SC-SC) transformation solely through the loss and gain of crystallization solvent molecules. Structural characterization and studies performed on compounds **1-4** also included solid-state NMR (^1H, ^{13}C, ^{31}P); Fourier Transform Infrared (FT-IR); Elemental Analysis; Scanning Electron Microscopy (SEM); Energy Dispersive X-ray Spectroscopy (EDS); Electron Microscopy EDS mapping and Protonic Conductivity [1].

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P19

NOVEL IONIC LIQUIDS: A SYNTHESIS TOWARDS SENSING ABILITIES

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Keywords: Ionic Liquids, Sensors, Target Analytes

In the last few decades, ionic liquids (ILs) have received quite a particular amount of attention from the scientific community as well as from the industrial field. This interest can be oversimplified by their typically inherent interesting physicochemical properties. Usually characterized by having high thermal stability, particular electrochemical properties, negligible vapor pressure and limited solubility in various solvents, with almost endless applications in both scientific and everyday use, these are enough arguments for such attention. These features have prompted their usage in organic synthesis[1] and in the preparation of new material (coordination polymers)[2], capacitors[3], solar[4] and fuel cells[5], among several other applications. Nevertheless, the typical cost of production is the most noticeable drawback attributed to ILs; therefore, in order to belittle this, our group is interested in developing inexpensive novel ionic liquids with added value.

It is our objective to amperometrically detect specific analytes which, in aqueous media, is difficult to do so, either by insolubility issues or by masking of the water specific redox behaviour.

Until this moment, new ILs have been synthesized, their chemical/electro-chemical characterization has been performed and pre-testing is underway. Simultaneously, computational calcula-tions for the assessment of their optical properties are being carried out and the possibility of obtaining new derivatives is being evaluated.

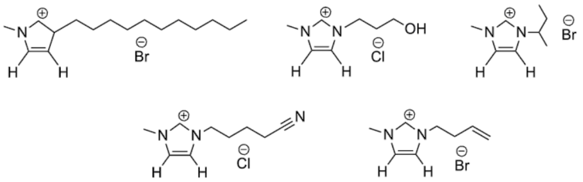

Figure 1: Structures of some of the synthesized ILs.

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P20

SUPPORTED IMIDAZOLIUM-BASED IONIC LIQUIDS: NEW MATERIALS FOR THE ADSORPTION OF ANTI-INFLAMMATORY DRUGS

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Keywords: Non-Steroidal Anti-Inflammatory Drugs, Supported Imidazolium-Based Ionic Liquids, Adsorption.

Diclofenac belongs to the non-steroidal anti-inflammatory drugs (NSAIDs), a class of active pharmaceutical ingredients (APIs) used in hospitals and as veterinary drugs. NSAIDs provide analgesic and antipyretic effects, and in higher doses, anti-inflammatory effects, where prescription is not needed, and therefore, they are denominated as “over the counter” drugs. However, due to their large consumption, NSAIDs are found in aqueous streams in concentrations ranging from ng/L to µg/L,[1] leading thus to serious concerns in the public health. Albeit STPs and WWTPs use advanced technologies for the removal of pollutants/contaminants, none of those methodologies was specifically designed for APIs, explaining why some of these contaminants were already detected even in drinking water.[1]

This work addresses the preparation of novel materials, based on silica modified with 1-methyl-2-propylimidazolium ($[C_1C_3im]^+$) for removal of diclofenac from aqueous media. The modified silica ($[Sil][C_1C_3im]X$) was characterized by infrared spectroscopy, elemental analysis and ^{13}C solid nuclear magnetic resonance. Furthermore, the isotherms adsorption kinetics of the materials for diclofenac were measured. The adsorption equilibrium data obtained is well described by either Langmuir or Freundlich isotherm model. Outstanding results (up to 100% of adsorption efficiency) were obtained for the removal of diclofenac from aqueous media using the synthesized materials. Supported imidazolium-based materials are thus promising materials for the removal of active pharmaceutical ingredients and treatment of wastewater.

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FORENSIC DISCRIMINATION OF PLASTIC BAGS BY THERMAL AND SPECTROSCOPIC METHODS

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Keywords: forensic chemistry, plastic bags, polyethylene, discrimination

Plastic bags consist in a type of materials of interest for the forensic scientist that may be found in crime scenes. They can be used to hide useful proofs or other crime related materials, and to pack illicit drugs to be sold in the consumer market. [1-3]

In cases where illicit drugs are seized, one of the steps to follow is to try to correlate the seized plastic bags with unused bags, such as those found in the house of a suspect. Thus, it becomes useful to characterize these polymeric items in order to trace their source and obtain supplementary information that can help forensic investigations. [2,3]

In this work plastic bags were analyzed by differential scanning calorimetry, thermogravimetric analysis, polarized light microscopy, FTIR spectroscopy in transmittance and attenuated total reflection modes and X-ray diffraction. These methods allowed to study the formulation (polymer matrix and additives), structure (degree of crystallinity), microstructure (polymer chain) and morphology of plastic bags. [1]

Twenty-eight plastic bags collected from seven different brands were analyzed in three random sites. Inter and intra-sample variability of the same brand was investigated, along with the diversity among samples from different brands. Through the complementarity of these results it is demonstrated that it's possible to discriminate from apparently similar plastic bags, differences resulting from the manufacture process. [2-4]

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P22

GRAPHENE DERIVATIVES FOR CATALYTIC OZONATION

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Keywords: Graphene oxide, graphene oxide-TiO_2 composites, ozonation.

Nowadays, water and wastewater treatment and reuse become emphasized. Catalytic ozonation appears as one of the most promising advanced oxidation processes for water treatment. Carbon materials have been employed as catalyst supports and/or as catalysts on their own. In addition, heteroatoms, such as nitrogen (N) and sulphur (S) are known to affect the catalytic activity of carbon materials [1, 2]. The catalytic activity of N- and S- doped graphene-based materials for the degradation of oxalic acid by catalytic ozonation is investigated in the present work. The influence of TiO_2 on the performance of these graphene-based materials has been also assessed.

Graphene oxide (GO) was prepared by oxidation of synthetic graphite (Brodie [3] and Hummers [4] methods) followed by mechanical exfoliation (ultrasonication). N- and S- doped GO materials were produced by thermal annealing, respectively with ammonia gas [5] and benzyl disulfide [6], as precursors. Graphene derivatives-TiO_2 composites (GOT) were prepared by two methods, liquid phase deposition (LPD) [7] and simple mechanical mixture of TiO_2 and GO. The synthesized materials were characterized by XPS, SEM, nitrogen adsorption, elemental analysis and TGA. The metal-free carbon material prepared by the Brodie method, and doped with nitrogen, has a higher catalytic activity than the other tested materials. However, the GOT composite prepared by LPD presented a highest stability. Ozone has a strong erosive effect on the carbon phase, TiO_2 particles protecting the GO nanoplatelets.

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SILICA COATED GADOLINIUM NANOPARTICLES: SYNTHESIS AND CHARACTERIZATION

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Keywords: Silica nanoparticles; Nanotechnology; Magnetic resonance imaging (MRI)

One of the most important approaches of biomedical field is the development of new, effective and noninvasive medical diagnosis, and treatments that have such requirements as advanced technologies for tumor imaging. Gadolinium (Gd) compounds can be used as MRI contrast agents, however the release of Gd^{3+} ions present some adverse side effects such as renal failure, pancreatitis or local necrosis [1]. The present work proposes a strategy that combines therapeutics and diagnosis on a single platform. The main aim of the work was the development and optimization of Gd based particles coated with silica to be used as drug delivery and bioimaging agent. Gd based particles were prepared throughout a precipitation method where several temperatures and aging times were tested. Afterwards, these particles were covered by silica using the Stöber method. Physicochemical characterization was performed using Fourier Transform Infrared Spectroscopy (FT-IR) and X-ray Diffraction (XRD). The particles size and morphological characterization were carried out using Transmission Electron microscope (TEM). Results showed that temperature and aging time had a great influence in Gd nanoparticles preparation, where smaller nanoparticles were achieved with shorter aging times showing the narrowest size distribution. Regarding silica coating, results showed that nanoparticles were homogeneous regarding chemical composition, silica layer thickness, total size and morphology. In conclusion, our results showed that Gd based nanoparticles coated with silica for imaging and drug delivery applications were successfully produced by a well-controlled method.

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P24

SCANNING THERMAL MICROSCOPY: NANOSCALE MAPPING AND ACTING ON LOCAL (SUB)SURFACE THERMAL PROPERTIES

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Keywords: SThM, Nano-Thermal Analysis, Thermal management

The study of thermo-physical properties at the nano-scale is fundamental for understanding heat distribution in micro/nanostructured materials and miniaturized electronic, optoelectronic, thermoelectric, and sensing devices [1]. In this context, thermal nano-characterization techniques are required to address issues related to thermal management, such as localized self-heating and high operation temperatures, which compromise device performance [2]. Scanning Thermal Microscopy (SThM) is a probing technique based on an atomic force microscope (AFM) whose main feature is a specialized heated thermal nano-probe designed to act as thermometer and resistive heater, achieving the high spatial resolution required for thermal studies at micro and nanoscales [3-4]. This contact technique provides simultaneous collection of surface topography and thermal data, which enables direct observation and mapping of thermal properties such as thermal conductivity, temperature and thermal contact resistance between dissimilar materials. SThM has become a powerful tool with a leading role in diverse fields of science and engineering [5].

We present the contribution of SThM in several relevant research topics: 1) studies of thermal conductivity contrast in graphene monolayers deposited on different substrates were conducted. SThM proves itself a reliable technique to clarify the intriguing thermal properties of graphene which, due to its high efficiency in heat conduction, is viewed as an important contributor to minimize performance issues ensuing from devices and materials downscaling. 2) SThM's ability to perform sub-surface imaging, by presenting thermal conductivity contrast analysis of polymeric composites showing detailed sub-surface features of the material which are unobservable through surface topographical analysis. 3) Nano-Thermal Analysis inducing local structural transitions to determine the corresponding transition temperatures in ferromagnetic shape memory alloy Ni-Mn-Ga thin films. This study consists in locally heating the sample and observing the material's local structural changes (characterized by discontinuities in cantilever deflection) while measuring the temperature at which such transformations occur. Mapping of local structural transition temperatures was performed and it is shown to be consistent with temperature dependent AFM analysis and the material's phase diagram. 4) Studies on heat absorption and release in phase change materials (PCM) as latent heat storage resources.

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g-C_3N_4 MODIFIED BY THERMAL, CHEMICAL AND MECHANICAL ROUTES FOR THE SELECTIVE PHOTOCATALYTIC SYNTHESIS OF BENZALDEHYDE FROM BENZYL ALCOHOL

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Keywords: selective photocatalytic oxidation; benzaldehyde; carbon nitride.

Benzaldehyde is a chemical of great importance due to the wide variety of industrial applications, including fine chemistry and the manufacture of polymers, fragrance compounds, dyes and pharmaceutical ingredients [1].

Seeking for a reduction of the environmental footprint in the production of consumables, in the present work, the selective photocatalytic conversion of benzyl alcohol to benzaldehyde was studied in aqueous medium (instead of using organic solvents). The combination of environmentally friendly conditions (metal-free catalysts based on graphitic carbon nitride, g-C_3N_4, natural pH, ambient temperature and pressure, and light emitting diodes (LEDs) as highly efficient lighting source) was also attempted.

Bulk g-C_3N_4 was synthesized by thermal condensation of dicyandiamide, and post-treated by thermal (T), mechanical (M) and chemical (C) routes. The effect of the temperature (400, 450 and 500 ºC), time of mechanical treatment (1.5, 3.0 and 8.0 h) and acid (H_2SO_4, HCl and HNO_3) employed, on the conversion of benzyl alcohol and the selectivity and yield towards benzaldehyde, was investigated. Results show that post-treatments can significantly enhance photocatalytic conversions and yields, the selectivity slightly decreasing. The most promising catalyst was that post-treated at 500 ºC which has the highest BET surface area (87 m^2 g^{-1}) achieving 66% conversion, 59% yield, and 90% selectivity. The catalysts were further characterized in order to investigate possible effects on their photocatalytic performance.

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DEVELOPMENT AND CHARACTERIZATION OF INNOVATIVE BIONANOCOMPOSITES BASED ON POLYSACCHARIDES AND PROTEIN NANOFIBERS

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Keywords: Protein nanofibers, Polysaccharides, Bionanocomposites

The production of chemicals, materials, fuels and energy is nowadays progressively moving in the direction of renewable resources, and there is a growing interest on the use of polysaccharides, such as cellulose, pullulan and chitosan for the development of new sustainable materials with distinct functionalities and applications. Proteins are also gaining increasing attention as singular components for multi-functional biomaterials. The assembly of proteins into long and insoluble ordered fibrillar structures (protein nanofibers) is a very recent and promising strategy for the development and characterization of nanosized reinforcing elements for bionanocomposites, with applications ranging from medicine to soft matter and nanotechnology.

In this project, proteins, such as insulin, β-lactoglobulin and hen egg white lysozyme, were fibrillated and combined with different polysaccharides, namely pullulan and cellulose (both vegetal and bacterial forms) to develop new functional biomaterials such as films and aerogels for application in the biomedical field. These new functional biomaterials were characterized in terms of morphology, biocompatibility and mechanical properties (Young's modulus), as well as cell adhesion and proliferation and its potential to be used as scaffolds in the biomedical field.

BACTERIAL CELLULOSE-BASED ELECTROLYTES FOR SOLID ALKALINE FUEL CELLS

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Keywords: Bacterial Cellulose, Anion Exchange Membranes, Solid Alkaline Fuel Cells

Bacterial cellulose (BC) is a highly pure and crystalline form of cellulose produced by bacteria directly with a three-dimensional, cross-linked nano- and micro-fibrilar structure that confers it excellent mechanical properties [1].

BC is naturally formed as mats that are readily available to produce novel bio-based composites that combine the BC enhanced thermo-mechanical behavior with other functional properties.

our group recently proposed BC as backbone materials for proton conducting membranes through the free radical polymerization of a polyelectrolyte directly inside BC mats [2].

Here we describe a similar method to produce BC-based anion conductive membranes by forming nanocomposites with a polyelectrolyte. The objective is to produce a green material combining the thermo-mechanic characteristics of BC and the anionic conductivity of poly(3-acrylamidopropyl) trimethylammonium hydroxide.

Nanocomposite membranes with variable thickness from 80 to 400 μm and defects free were obtained. The composites are thermally stable up to 200 °C, close to what is observed for pure BC. The composites present also a lower storage modulus than BC, attaining nevertheless more than 1 GPa and revealing that the viscoelastic behavior of pure BC is maintained.

The in-plane anionic conductivity achieved, 7.61×10^{-2} $S.cm^{-1}$ at 94 °C / 98% RH, is lower than for typical proton conductive membranes, but a top figure for anion exchange membranes.

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IMMOBILIZATION OF LACCASE OVER NANOMATERIALS FOR OXIDATIVE BIOCATALYSIS

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Keywords: laccase, immobilization, nanomaterials

Enzyme immobilization over solid carriers is of crucial importance in industrial applications since it allows multiple reuse and increase stability of the valuable enzymes, thus reducing the process costs. Recent developments in nanotechnology provided access to novel materials with unique structures and properties, which may present enormous advantages when acting as carriers for enzyme immobilization: large specific surface area, high adsorption and enzyme loading capacity, low mass transfer resistance and the ability to be functionalized. We have recently demonstrated how magnetic nanoparticles (MNPs) and multiwalled carbon nanotubes (MWCNTs) can be used as carriers for laccase immobilization [1,2]. These materials were thoroughly characterized by microscopic and spectroscopic techniques, including TEM, FTIR and BET specific surface area determination. The catalytic activity of immobilized laccase was evaluated towards 2,2-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid (ABTS) oxidation.

The characterization results showed that laccase was successfully immobilized over both nanomaterials. However, the optimal pH condition for immobilization depended on the carrier. A comparative study will be presented for the performance of the enzyme when immobilized over the two different carriers. The kinetic parameters and the operational stability showed that laccase had a lower affinity to the ABTS when immobilized on either nanomaterial, but it was possible to reuse the bioconjugate in several consecutive cycles, which represents an important advantage for industrial applications.

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CONDUCTING AND PARAMAGNETIC PROPERTIES OF d-PCL(530)/SILOXANE-BASED BIOHYBRIDS DOPED WITH MANGANESE PERCHLORATE

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Keyword(s): biohybrids, paramagnetism

Polymer electrolytes (PEs) have attracted much interest to the scientific community because of their technological application in the domain of solid state electrochemistry, in particular for the fabrication of advanced batteries, sensors, photoelectrochemical, and electrochromic devices (ECDs). Actual research on solid-state electrochemistry seeks a compromise between “green” technologies, low cost, and highly efficient materials.

In the framework of the investigation of new “green” materials with improved properties and potential application as electrolytes in ECDs, several ormolyte (organically modified silicate electrolyte) systems composed of a sol-gel derived poly(ε-caprolactone) (PCL(530), where 530 represents the average molecular weight in g mol^{-1})-based di-urethanesil hybrid network (abbreviated as d-PCL(530)/siloxane) have been tested in the last few years [1-3].

In the present work, the d-PCL(530)/siloxane biohybrid was doped with manganese perchlorate ($Mn(ClO_4)_2$), where the incorporation of Mn^{2+} ions has a two-fold interest, endowing the resulting hybrids with ionic conductivity and specially paramagnetic properties. The structure, morphology, thermal features, ionic conductivity, and paramagnetic properties of the $Mn(ClO_4)_2$-doped d-PCL(530)/siloxane biohybrids are presented in this communication.

The prepared material with the best conductive performance presented ionic conductivity values up to 4.8×10^{-8} and 2.0×10^{-6} S cm^{-1} at about 25 and 100 ºC, respectively. FT-IR data demonstrated that the hydrogen bonding interactions present in the non-doped d-PCL(530)/siloxane host hybrid matrix were significantly influenced by the inclusion of $Mn(ClO_4)_2$ which promoted the formation of more oxyethylene/urethane and urethane/urethane aggregates. In addition, the Mn^{2+} ions bonded to all the “free” C=O groups of the urethane cross-links and to some of the “free” ester groups of the amorphous PCL(530) chains. The magnitude of the electron paramagnetic resonance (EPR) hyperfine constant of the analyzed samples ($A \approx 90\times10^{-4}$ cm^{-1}) suggested that the bonding between Mn^{2+} ions and the surrounding ligands is moderately ionic. The synthetized d-PCL(530)/siloxane$_n$$Mn(ClO_4)_2$ biohybrids have potential application in paramagnetic, photoelectrochemical and electrochromic devices.

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LOW-COST UPCONVERSION QUANTUM YIELD MEASUREMENT SETUP

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Keyword(s): Emission quantum yield, integrating sphere, upconverting nanoparticles.

Photon upconversion refers to a nonlinear optical process characterized by the successive absorption of two or more pump low-energy photons (usually in the near-infrared, NIR, spectral region) followed by the emission of output radiation at shorter wavelengths (higher energy) [1,2]. This unique form of spectral conversion has received much interest in areas such as biological imaging [3], telecommunications [4], and photovoltaics [5]. However, to evaluate the potential applicability of upconverting materials, it is required the knowledge of the light output efficiency under a given excitation wavelength. The upconversion effectiveness may be accessed by the emission quantum yield (q) defined by the ratio between the number of emitted photons and the number of absorbed ones.

The present work describes the implementation of a simple and low-cost quantum yield measurement setup using a commercially available integrating sphere-based spectrometer operating in the visible spectral range. This system was coupled to a power meter that enabled the determination of the incident number of operating in a broad spectral region ranging from the visible to the near-infrared. The performance and reliability of the developed setup was tested measuring the emission quantum yield values of well-known down-shifting and upconverting phosphors.

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SYNTHESIS AND CHARACTERIZATION OF ERBIUM-DOPED YTTERBIUM ALUMINIUM GARNET (YbAG:Er) FOR OPTICAL THERMOMETRY

P31

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Keywords: Optical thermometry, YbAG:Er, Solution Combustion Synthesis, Laser Floating Zone

A kind of optical thermometry method is the fluorescence intensity ratio technique, based on the measurement of fluorescence intensities ratios from two thermally coupled excited levels that, being independent of spectrum losses and fluctuations in the excitation intensity, leads to a high accuracy of the material temperature measurement. Just some materials, mainly triply ionized RE ions imbibed in an appropriate host, obey the needed requirements to act as a thermal sensor being Erbium-doped ytterbium aluminum garnet (YbAG:Er) one of them [1].

We report the successful production of YbAG:Er by two different techniques: nano powders by Solution Combustion Synthesis (SCS), using a mixture of two fuels (urea and glycine) and fibers by Laser Floating Zone (LFZ) grew using oxides of the same reagents used in the SCS technique as precursors.

The structure and relevant optical properties of the prepared materials has been confirmed and characterized by X-ray powder diffraction (XRD), Raman spectroscopy (RS), absorption and photoluminescence (PL). XRD results show that the both powders and fibers are single phase YbAG in which the introduction of the Er trivalent ions did not distorted the network symmetry. Raman spectroscopy corroborates these results. Room temperature PL results confirm the introduction of the Er^{3+} ion in the host lattice and its optical activation as well as, when excited with a 980 nm diode laser, the existence of up-conversion mechanisms with emission in the expected violet, green and red spectral range depending on the excitation power. The influence of post synthesis annealing of the produced powders were also studied indicating a crystallite size increase with the anneal temperature and that no other phases of the ternary system, Al_2O_3-Yb_2O_3- Er_2O_3, are formed at the studied temperatures.

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CARBON DIOXIDE CAPTURE BY ENCAPSULATED IONIC LIQUIDS

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Keyword(s): Carbon Dioxide; Ionic Liquids; Encapsulated Ionic Liquids; Carbon Submicrocapsules

Due to their potential, ionic liquids (ILs) have been widely investigated during the last years for carbon dioxide (CO_2) capture aiming industrial applications. Despite presenting outstanding properties, some limitations are also existent, such as those related to transport properties [1].

This work presents a novel material called encapsulated ionic liquids (ENILs), consisting of IL introduced into carbon submicrocapsules [2], capable of overcoming these known limitations and transport properties of ILs to suitable solvents for Carbon Capture and Storage (CCS) industrial applications. These ENILs contain 80% w/w of IL, but discretized in submicroscopic encapsulated drops, drastically increasing the surface contact area with respect to the neat fluid [3]. This material will be applied to the removal of CO_2 from gas effluent.

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EFFECT OF HEAT TREATMENT ON THE COLORIMETRIC PROPERTIES AND THERMAL DEGRADATION OF *Eucalyptus urophylla* WOOD

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Keywords: Thermal treatment, thermorretification, colorimetry, thermogravimetry

Thermorretification, or thermal treatment, is a process to treat wood without the use of chemical products that consists in exposing the material to high temperatures (up 250ºC) [1]. That treatment causes a change in colour, making a common wood look similar to an expensive tropical wood. It also provides an improved dimensional stability and more resistance to xylophagous fungi.

In this work, wood samples from the MN-463 clone (natural hybrid of *Eucalyptus urophylla*) were treated at different temperatures, in order to evaluate the effect of temperature on the colorimetric properties, and the thermal degradation of the treated wood. Samples were heated in an oven at 140, 160, 180, 200, 220 and 250 ºC for 3 h. Thus, each material was subjected to 6 different treatments, apart from the blank sample, and each procedure was repeated 20 times. The following colorimetric parameters were evaluated: clarity (L*), red shade (a*) and yellow shade (b*), based on the CIELAB 1976 colour scale. The thermal degradation was evaluated by thermogravimetric analysis (TG/DTG), as commonly made [2].

It was shown that both clarity (L*), red shade (a*) and yellow shade (b*) were reduced above 160 ºC and that 250ºC was the temperature that generated the largest residual mass. The increase in temperature was effective for colour change (Figure 1). TG/DTG showed that the weight loss was smaller for woods previously treated at higher temperatures.

Figure 1 – Colour changes in wood caused bv different thermal

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PRELIMINARY SEM STUDIES ON NORMAL AND ALTERED GONADS OF *CATOSTYLUS TAGI*

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Keywords: symbionts of *Catostylus tagi*, marine parasites, SEM of gonads

Nowadays,_due to concerns about climate change, there is an increasing interest in the role of jellyfish in ecosystems; these studies have shown a close interaction among jellyfish, fishes and other taxa. The interactions between such marine organisms are complex and dynamics. It is known that according to the life stage, they can change from mutualism to commensalism and vice-versa; even parasitism can be shared [1].

Catostylus tagi is an edible Scyphozoa, and the sole European Catostylidae, which occurs in summer at Tagus and Sado estuaries. In view of its application in health sciences, some aspects about this jellyfish have already been studied [2]. To start the study of its life cycle, exemplars were collected to characterize the sex and gonads stage by optical (OM) and scanning electron microscopy (SEM).

The intact cells of female were regular spheres with a mean diameter of 31 µm (n = 400) in September. In the same period, the healthy male cells were more abundant, with a somewhat irregular elongated shape and smaller (24 µm, n = 400). No correlation was found between the sex and the colour of the gonad (green or brown or yellow).

The observations at the gonads of *C. tagi* by SEM exposed some cells with ruptured walls and at least two other organisms, a crustacean and a cnidarian. The crustacean could be *Hyperia gaudochaudii*, already mentioned in *C. mosaicus*, an Australian jellyfish, although without images available [3]. The cnidarian had morphological similarities with *Polypodium hydriforme* which is known to parasite the gonads of fish belonging to the family Acipenseridae, commonly named sturgeons [4]. As both *C. tagi* and the sturgeons are estuarine animals, it is not absurd that they share the same parasite. Genetic studies through amplification of genomic DNA (18S rDNA) of the organisms are now in progress.

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DEVELOPMENT OF AN INTEGRATED OPTICAL DEMODULATOR FOR COHERENT SYSTEMS

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Keywords: 90º hybrid coupler, di-ureasil and demodulator

The continued growth of information transmitted daily requires the development of optical components that support high bandwidth [1]. Within optical communications technology, coherent optical systems are highly interesting because they allow a variety of modulation formats. However to implement this type of optical systems it is required several devices, such as optical signal modulators and demodulators, which have a high production cost. This work focus in the Quadrature Phase Shift Keying (QPSK) modulation, which duplicate the information transmission capacity, using the optical signal phase to encode the data [2].

In order to reduce the cost of optical components for optical communication, in this work, it was develop devices based on organic-inorganic hybrids to demodulate a QPSK signal. It is demonstrated the implementation of an integrated optical coherent receiver based on a 90° hybrid coupler, manufactured with UV laser patterned method in the surface of organic-inorganic di-ureasil hybrids. The 90° hybrid coupler was designed and optimized, revealing propagation in the NIR spectral region. The device shows an input – output ports transfer function that is dependent of the optical signal phase, being therefore able to demodulate a QPSK signal. To demodulate the QPSK signal automatically, the results were recorded, and the phase difference information from the video was obtained using a MATLAB program, that was develop for this purpose.

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WATER-FREE NEODYMIUM 2,6-NAPHTHALENEDICARBOXYLATES COORDINATION COMPLEXES FOR ISOPRENE POLYMERIZATION

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Keywords: neodymium, metallic organic frameworks (MOFs)

A series of four coordination polymers based on neodymium have been hydrothermally synthesized with different carboxylic acids as a linker. The structures of the compounds $Nd_2(2,6\text{-ndc})_3(H_2O)_3{\cdot}H_2O$ (1), $Nd_2(2,6\text{-ndc})_2(ox)(H_2O)_2$ (2), and Nd(2,6-ndc)(form) (3) (2,6-ndc = 2,6-naphthalenedicarboxylate; ox = oxalate; and form = formate) have been determined by single-crystal X-ray diffraction analysis. 1-4 exhibit rather dense networks built up from infinite chains of NdO polyhedra connected to each other through the 2,6-ndc ligand. Terminal and bridging aquo species are present in the coordination sphere of Nd for 1, whereas some of them are partially replaced by oxalate groups in 2 and fully substituted by formate groups in 3.

The water-free phase 3 as well as the compound $Nd(form)_3$ (4) were considered for catalytic reaction for polymerization of isoprene in the presence of Al-based cocatalyst, affording cispolyisoprene with good conversions. Residual Nd material with unchanged structure was found in the polymeric material by comparison with scanning electron microscopy and powder X-ray diffraction. The neodymium luminescence of compounds 3 and 4 was also measured by FT-Raman.

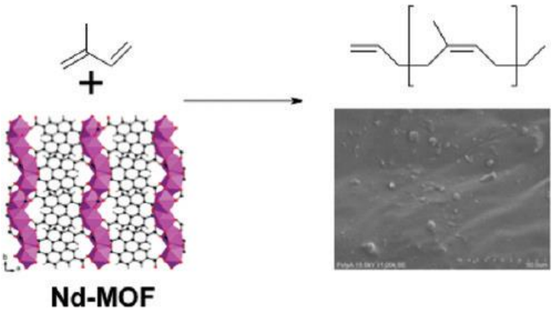

Figure 1. Polymerization of isoprene by 3. View of the 3D structure of 3 along the *c*-axis, showing the connection of the mixed organic – inorganic layer Nd(2,6-ndc)(form) through the 2,6-ndc ligand (bottom left) and SEM images of the polyisoprene surface produced with 3 (bottom right).

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POLYBENZIMIDAZOLE POLYMER CONDITIONING FOR GENOTOXIC IMPURITIES REMOVAL FROM ACTIVE PHARMACEUTICAL INGREDIENTS POST REACTION STREAMS

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Keywords: PBI Adsorbents, genotoxic removal.

During the process of synthesis of active pharmaceutical ingredients (API) it is common the presence of impurities in the final product derived from the presence of by-products, inefficient removal of catalyst, unused reactive reactants added in molar excess and traces of organic solvents [1]. These impurities, if intaken by patients, may have several side effects including reacting with DNA preventing its normal replication. In the later case, such impurities are classified as being genotoxic impurities (GTI). The concern of pharmaceutical industries with the presence of GTIs in API is calling for development of processes that respect the GTI limits established by regulatory agencies, while reducing the loss of API during the purification steps [2]. In this work we report the use of thermally treated and acid or alkaline conditioned of polybenzimidazole (PBI) polymer as methods to improve PBI affinity to remove the GTIs methyl p-toluene sulfonate (MPTS) and 4,4-dimethylaminopyridine (DMAP) from Mometasone furoate (Meta) API stream. This new material demonstrated high efficiency removals for both GTIs in concentrations up to 1000 ppm with API losses less than 10%.

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CHARACTERIZATION OF A W-(Sn) SKARN ORE TO IDENTIFY POSSIBLE MINERAL PROCESSING OPTIONS

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Keywords: mineralogy, skarn, processing

The “Scheelite Tungsten Belt”, Northern Portugal, is characterized by the occurrence of W mineralized skarn horizons, which are currently being investigated under the scope of the Horizon 2020 project **FAME** (Flexible and Mobile Economic Processing Technologies - 641650 - H2020 - SC5 - 2014) with the aim to carry, in a near future, their efficient exploitation and ore processing.

The mineralogy of the skarns is well-known comprising vesuvianite, fluorite, scheelite, calcite, apatite, quartz, plagioclase, K-feldspar, epidotes, pyroxene, sericite, garnet, amphibole, cassiterite and rare sulphides (sphalerite and arsenopyrite). A previous observation with UV lamp revealed the scheelite (blue fluorescent) and also a yellow- fluorescent mineral, assumed as a calcium molybdate (powellite). This fact raised the authors’ attention, since geochemical analysis of the deposit by ICPMS revealed the absence of Mo. In order to investigate the characteristics of scheelite and clarify the existence or not of powellite, petrographic examination in transmitted polarized light was complemented by scanning electron microscopy (SEM), Raman spectroscopy and electron microprobe analysis.

The petrographic examination allowed identifying scheelite crystals with different sizes: very fine-grained (< 60 µm) and fine (60 to 250 µm) crystals; and medium (250 to 500 µm) and coarse-grained (> 500 µm) poorly rounded assemblages of crystals. The finer crystals seem to cluster in order to form the coarser grains. The different scheelite types reveal identical composition corresponding to members with very low Mo content (0.05 to 0.09%).

As for the fluorescent mineral, a bipyramidal-shape crystal (up to 400 µm) included in vesuvianite was identified under the petrographic microscope. The investigated mineral is replaced by cassiterite, fluorite, quartz and calcite. Raman spectroscopy revealed a spectrum compatible with the one of the tin silicate malayaite ($CaSnSiO_5$), which, till now, was never described in Portuguese lithologies, though it is a common in tin deposits around the world. The semi-quantitative and quantitative compositions of these minerals were obtained using SEM and the electron microprobe, respectively. In some crystals, both EDS and WDS analyses confirmed the presence Al, Fe and Ti in the mineral’s structure, which is indicative of minerals belonging to the solid solution titanite-malayaite. Stokesite ($CaSnSi_3O_9.2H_2O$) was also identified in microcracks cutting vesuvianite.

The combined use of all these characterization techniques allowed the successful characterization of the skarn ore, thus contributing to a better knowledge of its mineralogy and to identifying subsidiary tin ore minerals to be potentially exploited and processed besides scheelite.

UNPRECEDENTED DETAILS ON THE SURFACE STRUCTURE OF CO_2 SPECIES IN MESOPOROUS MATERIALS USING SOLID-STATE NMR AND MODELING

P39

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Keywords: $^{13}CO_2$ capture, mesoporous materials, solid-state NMR

The quest for new materials aiming to extract carbon dioxide from power plant flue gas streams or from exhaled air in *life support* systems in spacecrafts makes the study of CO_2 speciation in amine-tethered porous sorbent materials an extremely attractive research topic. In order to reduce the high concentrations of CO_2, adsorbent materials have been studied for CO_2 capture in replacement of liquid-phase amine adsorbents, to overcome the inherent corrosion and low energy efficiency issues related with the use of aqueous amine solutions [1-3].

Despite of the numerous contributions, understanding the stability and chemical nature of CO_2 species formed at the material surface is still a difficult challenge where sophisticated spectroscopic studies are lacking. Mesoporous silicas, such as SBA-15, reported in this work, functionalized with amines are among the most relevant materials being developed [1,3] due to their high selectivity and capacity toward CO_2 at low partial pressures [2,3]. In these materials, the mechanism of CO_2 capture by the amines is assumed to be essentially the same as in aqueous amine solutions, but we show that this assumption is not correct and that the nature of the grafted amines, silica substrate and amine density strongly influences the nature of the CO_2 species present. The present work comprises solid-state NMR and computational studies of various functionalized SBA-15 silicas with primary and secondary amines loaded with ^{13}C-labeled CO_2, under controlled partial pressure, to characterize the chemisorbed CO_2 species [3]. A combination of 1D and 2D ^{13}C-based MAS NMR experiments were performed in as-prepared and H/D exchanged SBA-15 showing that the CO_2 species are engaged in very complex hydrogen bonding networks. Distinguishing between CO_2 species based on carbamic acid (neutral) and alkylammonium ion pairs (deprotonated charged species) generated at the pore surface has been a longstanding problem. Herein, we report for the first time a method sensitive to proton transfer based on chemical shift anisotropy (CSA) tensor analysis on strategically designed mesoporous silicas with controled amine separation.

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BUNDLE STRUCTURE OF HOLLOW-CORE TRIANGULAR LUMINESCENT SOLAR CONCENTRATORS BASED ON VISIBLE AND NIR EMITTING TRIPODAL ORGANIC-INORGANIC HYBRIDS

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Keywords: luminescent solar concentrators, organic-inorganic hybrids, visible and NIR emission

Luminescent solar concentrators (LSCs) appear as an interesting way to cope with the limitations of commercial photovoltaic (PV) devices, namely the mismatch between its response and the solar spectrum, with the additional advantage of facilitating the integration of photovoltaics into the urban environment [1-3]. The most common PV cells are based on crystalline silicon (c-Si), which have larger external quantum efficiency (EQE) in the NIR spectral region, thus, LSCs emitting in such region are desired. Ideally they should absorb in the ultraviolet-blue region of the solar spectrum and emit in the NIR region [4], allowing the creation of transparent window panels providing natural lighting or a clear view and, also, solar radiation harvesting. Here, it is presented a new geometry for LSCs based on hollow-core plastic optical fibers, filled with organicinorganic hybrid materials doped with Rhodamine 6G, an Eu^{3+}-beta diketonate complex and Rhodamine 800, conferring visible and NIR emission to the active layers. The triangular shape of the LSCs allows an easier coupling of the LSCs into a bundle structure, posteriorly coupled to a Si-based commercial PV cell and characterized in terms of the PV cell EQE gain. An increase on Si PV cell EQE values is observed in agreement with the excitation spectra of the active layers, with an absolute EQE increase of ~50 % in the 300-400 nm range, higher than the record value reported for a downshifting layer based on Lumogen 300 organic dye dispersed in poly(methylmethacrylate) on a Si PV cell [5].

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IDENTIFICATION AND CHARACTERIZATION OF C-NANOPARTICLES AND NANOMINERALS FROM COAL COMBUSTION BY HR-TEM/EDX

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Keywords: coal mining, spontaneous combustion, carbon-containing particles

The coal combustion for power generation and the spontaneous combustion of coal wastes are a potential source of nanoparticles in resulting by-products. The importance of the study of carbon nanoparticles is related with the development of nanotechnology that has been attracting attention due to the ability of these materials to be used in different technologies such as electronic, biomedical, pharmaceutical, energy, material applications, etc. Most attention should also be dedicated to environmental and health implications of nanoparticles from combustion processes. Previous studies demonstrated that carbon nanotubes, fullerenes, other C-containing nanoparticles and nanominerals have been identified in various geological materials, including coal and its combustion by-products [1, 2]. The main goal of this work is the identification and characterization of nanoparticles (organic and inorganic) present in materials thermally affected by spontaneous combustion process in coal waste piles resulted from coal mining. Samples of non-thermally affected coal samples were also analyzed for identification of changes caused by the combustion process. The studied samples are from Douro Coalfield (NW of Portugal) and from El Bierzo Coalfield (NW of Spain). High resolution transmission electron microscope with energy-dispersive x-ray spectroscopy (HR-TEM/EDX) was used for the identification and characterization (size, shape, morphology, microstructure, chemical composition and crystallinity) of the carbon containing geological samples. For HR-TEM/EDX analyses the samples were firstly powdered, suspended in water, and then were prepared by drop casting the solutions on cupper grids coated with amorphous carbon ultrathin films and left to dry at room temperature. The HR-TEM/EDX observations and analyses demonstrated that the coal, coal waste material, present a wide variety of carbon constituents with different aspects, structure, and size. Carbon nanoparticles were identified in all the studied samples exhibiting some degree of crystallinity that seems to be more intense in burnt coal waste material which is attributed to the uncontrolled combustion process at high temperatures.

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DIFFERENT CHEMICAL ROUTES TO OBTAIN MAGNETIC NANOCOMPOSITES BASED ON EXFOLIATED GRAPHITE

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Keywords: exfoliated graphite; magnetic nanocomposites

The overarching objective of this research is to manufacture, characterize and apply graphite-based nanocomposites for multiple applications in the environmental field. The new nanomaterials produced will be used as adsorbents to remove toxic elements and compounds from water, as well as to recovery scarce trace elements used as key components for the development of new technologies (the so-called technology-critical elements).

In this presentation the major focus will be given to the synthesis of magnetic exfoliated graphite nanocomposites by two different chemical routes and to their full characterization. The two chemical routes adopted were (i) the sonication of exfoliated graphite (EG) in the presence of magnetite nanoparticles (Fe_3O_4 NPs) and, (ii) the *in situ* oxidative hydrolysis of Fe(II)SO_4 in alkaline media. The nanocomposites denoted, respectively, by Fe_3O_4@EG01 and Fe_3O_4@EG02, were then fully characterized (scanning electron microscopy (SEM), transmission electron microscopy (TEM), Raman spectroscopy, Fourier Transform Infrared Spectroscopy (FT-IR), vibrating-sample magnetization (VSM) curves, X-Ray powder diffraction; Fe concentration, zeta potential, and Boehm titration) in order to select the best material for the practical applications proposed.

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OPTICAL, STRUCTURAL, MORPHOLOGICAL AND ELECTROCHEMICAL PROPERTIES OF NANOSTRUCTURED MN DOPED CEO_2 THIN FILMS PROCURED BY SILAR

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Keywords: metal-oxide, pseudocapacitance, cerium oxide, doping, manganese, SILAR

Nanostructured metal oxides (NMO), due to their diverse potential applications in fields of science and technology, have attracted significant attention in recent times [1]. Cerium dioxide (CeO_2) is not excluded and has been widely investigated as a new and promising pseudocapacitive material due to its prominent valence states and high interfacial charge transfer rate. Again, CeO_2 doped with metal ions (e.g. Mn, Cu, Fe, etc.) has exhibited intriguing novel properties in many aspects [2–4]. In the present study, nanostructured Mn doped CeO_2 thin films have been fabricated *via* successive ionic layer adsorption and reaction (SILAR) method. This method guarantees simplicity and versatility *cum* reproducibility of the NMO electrode material on various substrates. Mn doped CeO_2 of varying doping concentration (1, 3 and 5%) were successfully deposited on glass, FTO and silicon substrates and characterized using a multi-technique optical, structural, morphological and compositional approach. The feasibility of their application in supercapacitors is presented, as Mn doped CeO_2 electrodes showed a superior electrochemical richness compared to pristine CeO_2. Particularly, the cyclic voltammetry (CV) results confirmed a high specific capacitance of 690 Fg^{-1} for 5% Mn doped CeO_2.

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ELECTROSTATICALLY CROSSLINKED DNA/POLYCATION FILMS: A POTENTIAL DOXORUBICIN CONTROLLED RELEASE PLATFORM

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Keywords: DNA films, doxorubicin, controlled release

Films can be described as a layer or multilayer of one or more materials, having a thickness that may vary from the nano to the macro-scale. Films can be achieved through different methods, such as by immobilization of molecules on a surface by covalent conjugation or direct deposition (*e.g.* electrostatic interaction - layer-by-layer, cast films, UV irradiation crosslinking, etc.) [1]. For this purpose, a molecule of great interest is DNA due to its unique properties, and which has been used in several research fields [2]. Its negative charge allows it to electrostatically interact with opposite charged molecules, such as polycations, by self-assembly. Poly(amidoamine) (PAMAM) dendrimers, for example, are well known for being able to interact with DNA [3], mostly due to their protonated amine terminal groups at physiological pH. Here, we have successfully prepared DNA/polycation hybrid films, *via* electrostatic interactions, using PAMAM dendrimers of different generations (3, 4, 5) and 25kDa branched polyethyleneimine (PEI) under optimized experimental conditions. The films were characterized using several techniques - circular dichroism revealed a strong peak at around 300nm (revealing a case of gelation-induced supramolecular chirality) [4], their surface zeta-potential was positive, and scanning electron microscopy (SEM) showed that they had a homogenous interconnected granular surface. The films were quite stable over time, under physiological conditions (the free DNA in solution was dependent on PAMAM generation and serum content but, still, negligible). Films did not promote cell adhesion, but were not cytotoxic. Based on these results, we raised the possibility of applying the films as drug delivery platforms for doxorubicin (DOX), an anticancer drug. Taking advantage of DOX's ability to intercalate with DNA, DOX was loaded into the films with a high loading efficiency (around 85%) which was generation and polymer-independent. DOX release under physiological conditions showed a burst release in serum-free cell culture medium and a controlled release in other media (water, PBS and serum containing medium). Concluding, these DNA films may be interesting as drug delivery platforms.

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A VERSATILE TOOL FOR MOSQUITO REPELLENCY: SOLAR ACTIVATED RELEASE OF IR3535 FROM TiO_2 FUNCTIONALIZED-POLYURETHANE MICROCAPSULES

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Keywords: Photocatalysis, Microencapsulation, Titanium Dioxide

The main objective of this investigation is the functionalization of photocatalytic nanomaterials on the surface of polymeric microcapsules for the controlled release of encapsulated repellent compounds through solar radiation. The controlled release process is promoted upon solar radiation absorption by the action of reactive oxygen species produced during redox processes, as a result from the light-activated electronic inter-band transitions in the photocatalyst semiconductor material [1-3].

In this work, the active compound IR3535 was encapsulated in polyurethane microcapsules functionalized with titanium dioxide nanoparticles. I3535 is a synthetic insect repellent, well known for its great effectiveness to avert a number of insects such as mosquitoes and ticks and also for its low toxicological profile [4-5].

The TiO_2 nanoparticles were synthetized using a modified sol–gel coupled with a hydrothermal treatment, with a crystallite size of the order of 10 nm and a specific surface area >250 m^2/g. The effect of the nitrogen doping, time of synthesis reaction and hydrothermal treatment temperature was studied by photocatalytic experiments.

Functionalized-polyurethane microcapsules were prepared using a modified interfacial polymerization technique from the condensation reaction of an isocyanate and a polyol to form a polymeric film as microcapsule wall [3]. In vitro assays were carried out in insectaries at the Portuguese Institute of Hygiene and Tropical Medicine (IHMT), to test the efficiency and robustness of this novel photocatalytic microcapsule system to the prevention of mosquito-transmitted diseases. The results showed that functionalizing the microcapsules with nanoparticles on their surface and then exposing them to ultraviolet radiation effectively increased the output of IR3535 into the air, repelling the mosquitoes.

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GRAPHENE COATED TEXTILE WITH ELECTRICAL AND ANTIBACTERIAL PROPERTIES

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Keywords: electronic textiles, graphene, antibacterial

The development of electronic textiles is one of the hottest topics in organic electronics. There are already examples of smart textiles in garments for monitoring physiologic and biomechanical signals. However, manufacturing schemes for current applications rely on the integration of off-the-shelf electronic components mounted on a textile substrate. Such components are silicon-based, thus unsuitable for applications where flexibility and fault-tolerance are required. Organic electronics is an alternative to conventional silicon technology and can overcome these limitations. In this sense, graphene, with high optical transparency and electrical conductivity, is a promising material to be used as electrode. Graphene has also emerged as a novel green broad-spectrum antibacterial material, with little bacterial resistance. Furthermore, due to good biocompatibility, graphene-based nanocomposites with antibacterial properties have a wide range of applications, such as antibacterial packaging, wound dressing or water disinfection.

We recently developed an approach consisted in coating specially designed polypropylene and polylactide fibers with graphene and demonstrated that transparent monolayer graphene can coat textile fibers by wet transfer, forming a highly conductive thread with negligible change in transparency [1].

A graphene solution was also developed, based on ultrasonic exfoliation of graphite, which allowed textile coating by other solution methods such as drop cast and dip coating. Conductance of textile coated with graphene solution is lower than CVD graphene, yet it can be substantial improved by doping.

Finally, antibacterial activity against Gram-negative bacteria of textile with graphene and doped graphene has been evaluated. Particularly, graphene solution and graphene doped with HNO_3 and H_2O_2 alone and on textile exhibit antibacterial properties. On the contrary, graphene CVD and graphene doped with CsF, Cs_2CO_3 and CsF: Cs_2CO_3, alone and on textile, showed poor activity against bacteria, demonstrating graphene tunable antibacterial properties.

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CRYSTALLOGRAPHIC AND MAGNETIC CHARACTERIZATION OF LAYERED DOUBLE HYDROXIDES

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Keywords: Magnetic properties; layered double hydroxides

Layered double hydroxides (LDHs) are materials whose crystalline structure is built up from linked oxygen octahedra containing metal cations [1]. The general formula of the most common LDHs can be represented as $[M^{2+}_{1-x}M^{3+}_{x}(OH)_2]^{x+}(A^{z-})_{x/z}\cdot nH_2O$ where n is an amount of crystal water per formula unit. LDHs are composed of positively charged parallel hydroxide layers and charge-compensating anions A^{z-} intercalated into interlayer space. The interlayer distance can vary over a wide range depending on nature and orientation of the intercalated anions as well as on amount of crystal water.

The use of LDHs with different cationic and anionic content for various applications has been reported [2]. In particular, LDH materials containing magnetic transition metals (Fe, Ni, among others) can be potentially used as sustainable and recycled catalysts, adsorbents and ion exchangers. It has recently been shown that same specific distortions that modify magnetic order could appear in a framework of the face-linked octahedra [3]. This can be considered as a theoretical basis to discover new magnetic systems including those based on LDHs.

In this work, LDHs with different ratios of Co^{2+} as a bivalent cation to Al^{3+} as a trivalent cation ($[1-x]/x$=2,3 and 4) were prepared and intercalated with inorganic anions of different size and nature using co-precipitation. Crystal structure and crystallite morphology of the obtained LDHs were characterized using x-ray diffraction and transmission electron microscopy. Magnetic properties of these LDHs were quantified with superconducting quantum interference device and correlated with the interlayer distance and to the magnetic nature of the involved cations and their ratio in the hydroxide layers.

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INVESTIGATING FOREIGN MATERIAL IN PHARMACEUTICAL DRUGS: MORPHOLOGICAL AND ELEMENTAL ANALYSIS

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Keywords: pharmaceutical tablets, foreign material contamination, scanning electron microscopy

Contaminants detected during the drug manufacturing process present potential health risks to patient safety and may result in product release delays. Several recalls due to foreign material in solid dosage products have been widely reported in the past few years [1]. Therefore, it is of paramount importance to assure the absence of foreign material in drug product production by applying the most appropriate techniques in analytical laboratories.

In particular, the presence of foreign small particles at sub-visible size range (less than 100 μm) is of great concern since they cannot be easily detected. Different analytical techniques are available to identify and isolate such undesirable particles, allowing the identification of the contamination source and prevent future reoccurrences [1]. As example, the high resolution microscopic technique Scanning Electron Microscopy (SEM) coupled with Energy-Dispersive X-ray Spectroscopy (EDS) provides imaging data about the size, shape and morphology of the impurities, and also chemical identification based on the X-ray energy lines [2].

In this work, a case study that focus on the investigation of contaminated drug product tablets is presented. By applying SEM-EDS it was possible to characterize, isolate and identify the origin of impurities detected during a tablets production process development.

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Eu^{3+}-BASED BRIDGED SILSESQUIOXANES FOR TRANSPARENT LUMINESCENT SOLAR CONCENTRATORS

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Keywords: Bridged silsesquioxane organic-inorganic hybrids, lanthanide ions, luminescent solar concentrators

The conversion of solar energy into electricity through photovoltaic (PV) cells is not efficient enough and market competitive yet, remaining an obstacle for their large-scale dissemination. Luminescent solar concentrators (LSCs) are one way to improve the PV conversion efficiency in a cost effective way. LSCs are composed of films bearing optically active centers that collect the incident sunlight and reemit it partially at a specific wavelength. Part of this emitted light is trapped inside the layer and concentrated at the edge of the film where it can be collected by a PV cell.

Here, LSC will be produced using sol-gel derived bridged silsesquioxane containing Eu^{3+} salts and 2-thienoyltrifluoracetonate prepared from a new ethane tetracarboxamide-based organosilane [1]. Free-standing films with thicknesses up to 440 μm and maximum absolute quantum yield (q) of 0.34±0.03 (excitation at 320 nm) were prepared by the drop cast method, while thin films (~200–400 nm) spin-coated on glass substrates led to highly luminescent coatings with q=0.60±0.02 (excitation at 345 nm). The thin films were tested as LSC and the optimized device displays an optical conversion efficiency of 12.3% in the absorbing spectral region of the active layer (300–380 nm) [1].

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CARBON NANO-FILLERS LOADED POLYMERS FOR BLOOD CONTACT APPLICATIONS

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Keywords: Carbon nano-fillers | Composites | Hemocompatible | SEM | Tensile Properties

Blood-contacting devices (BCD) are applied either as external communicating devices (such as, cannulae or catheters) or implant devices (such as, heart valves or vascular grafts) for the diagnosis and treatment of several diseases. Most of the current devices commercially available are made of silicone, polypropylene, polyethylene terephthalate and polyvinylchloride which leads to several limitations in long-term usage, such as the occurrence of hemolysis, thrombosis, thromboembolic complications, immune responses, infection, and tissue overgrowth [1,2]. Due to the vital role of BCD, related complications have a high impact on the quality of life and survival of patients and also on health economy due to associated costs. All these facts, highlight an urgent need of new biomaterials for improvement of BCD performance. Thus, the aim of this work is to improve the mechanical properties of polymers by incorporation of carbon nano-fillers (CNFs) in order to evaluate their potential application in the design of BCD. Polymer/CNFs composites with different types and concentrations of CNFs were studied. CNFs incorporation led to a change in polymer color and surface topography, as observed by optical microscopy and scanning electron microscopy (SEM), respectively. Evaluation of the mechanical properties showed that upon incorporation of the higher CNFs concentration tested, the ultimate tensile strength of the polymer increased 2.5 times. However, SEM images revealed that human platelet adhesion and activation is very low in all materials, suggesting that it is not affected by CNFs incorporation. In conclusion, our study showed that CNFs have the potential to improve the mechanical properties of polymers, and despite changing the surface topography, the adhesion and activation of platelets are not affected.

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EVALUATION OF PHYSICAL STABILITY OF AMORPHOUS SOLID DISPERSIONS IN EARLY FORMULATION SCREENING

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Keywords: mDSC, physical stability, amorphous solid dispersions

Screening methodologies are typically used in early development of Amorphous Solid Dispersions (ASD) to select the appropriate polymer excipients and define the optimal drug load in the formulation.

Hovione has been applying a specific formulation screening methodology [1] that consists of three main stages:

- An initial miscibility assessment using in-silico simulations to assess phase separation propensity with different stabilizing carriers and drug loadings;
- Solvent casting trials with different stabilizing carriers and drug loadings to confirm the simulations. Solvent casting is done in DSC pans and after evaporation of the solvent the amorphous films are characterized by mDSC;
- Supersaturation studies to determine the most efficient polymers in maintaining high concentrations of drug in solution and inhibiting crystallization.

Characterization by mDSC of the amorphous films prepared by solvent casting is of paramount importance because it allows detecting key indicators of miscibility and phase separation of the cast films. Phase separation is an indication of physical instability and re-crystallization may be observed from the amorphous material. In general, a single T_g (glass transition temperature) indicates miscibility while the occurrence of a second T_g suggests immiscibility.

Two examples of solvent casting trials for formulation screening development are presented here. The results obtained in the mDSC show that the physical stability of amorphous films depends on both the type of polymer and polymer ratio used. Ultimately these results help deciding on the best formulation in terms of physical stability and are an important contribution towards selecting the best formulation.

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P52 IMPACT OF THE MANUFACTURING PROCESS ON THE MORPHOLOGY AND SIZE OF DRUG SUBSTANCE PARTICLES

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Keywords: Particle Size distribution, SEM, Laser diffraction

The control for particle size distribution and morphological particle properties (*e.g.*, shape, crystal habit, surface texture) of a drug substance are critical for maintaining the quality of drug products, in particular inhalation formulations [1]. These particle properties can have a direct effect on drug product’s properties and final performance. As example, cohesive and adhesive forces as well as drug-excipient interactions, that are dependent on particle morphology and surface, may influence product’s aerosolization and drug deposition in the target site.

This work aims to evaluate the impact of changes during the manufacturing process (e.g. grinding pressure and solids concentration) on the morphology and particle size of an inhalation drug substance, through techniques such as Laser Diffraction and Scanning Electronic Microscopy (SEM). The laser diffraction measurements help to understand the overall particle size distribution of the drug substance, while through SEM the individual size and surface morphology of the particles could be assessed. Data obtained allowed correlation of manufacturing conditions with particle features and, as a result, the optimization of the manufacturing process.

QUANTIFYING CRYSTALLINITY IN AMORPHOUS SOLID SOLUTIONS BY DSC

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Keywords: DSC, melting enthalpy, quantitative method, crystallinity

Polymorphism is a commonly encountered phenomenon in Active Drug Ingredients (API). The appearance or disappearance of a specific drug polymorphic form during manufacturing or storage is a major concern in drug process development. Thus rapid and reliable detection and quantification of polymorphic forms of API is essential during all stages of development [1]. Different analytical techniques, such as X-Ray powder Diffraction (XRPD), Infrared and Raman spectroscopy, Dynamic Vapor Sorption and thermal analysis, can be applied for this purpose. In fact, any solid state technique that can discriminate between different solid forms can be used to evaluate phase purity.

Differential Scanning Calorimetry (DSC) is a technique that measures the amount of energy absorbed or released by a sample when it is heated or cooled, providing quantitative and qualitative data on endothermic (heat absorption) and exothermic (heat evolution) processes. This information can be then used to quantitatively characterize solid solutions composition. For example, melting enthalpy is commonly applied for this purpose since this correlates with the concentration of the corresponding form in solution.

The work herein presented is intended to describe the methodology applied for the development and validation of a DSC quantitative method for the detection of crystalline active drug substance in an amorphous solid dispersion. Method was proven to be linear, accurate and precise with a limit of quantitation of 2.5% (w/w).

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ENHANCEMENT OF PHOTOVOLTAIC ENERGY CONVERSION BY DOWNSHIFTING WITH ORGANIC-INORGANIC HYBRIDS

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Keywords: Organic-inorganic hybrids, organic dyes, photovoltaics, down-shifting layers, external quantum efficiency

Organic-inorganic hybrids are promising candidates for a wide range of applications like fuel cells, optics, photonics, microelectronics and others [1]. However, their application as downshifting materials for photovoltaic (PV) cells has not yet been widely explored. The concept of down-shifting layers has been proposed as a method to improve the spectral response of solar cells to short-wavelength radiation, for example, the most used PV cells are Si-based with low performance for ultraviolet photons; and a way to significantly reduce the use of expensive semiconductor materials in photovoltaic energy conversion. The incorporation of organic-inorganic down-shifting layers in PV modules can provide a cheap and effective way to integrate photons conversion [2]. Down-shifting layers can be seen as distinct type of cost-effective devices easily integrated in PV energy conversion. Moreover, these devices can promote the integration of PV architectural elements into buildings, with the unprecedented possibilities for energy harvesting in façade design, urban furnishings and wearable solar fabrics. In this work, organic-inorganic hybrid (named as tri-ureasil) doped with organic dyes, such as rhodamine 6G, rhodamine 800 and silicon 2,3-naphthalocyanine bis(trihexylsilyloxide) will be used as down-shifting layers and the external quantum efficiency of Si PV cells will be evaluated.

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DIFFERENT APPROACHES FOR GRAPHENE INCORPORATION INTO POLYURETHANE

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Keywords: graphene, polyurethane, composites, coatings

Since its first isolation from graphite (Gt) in 2004, graphene (G) has attracted worldwide interest mainly due to its particular structure with hybridized sp^2 bonding. This structure confers G a hydrophobic and conductive nature as well as exceptional electronic, thermal and optical properties. Graphene based materials (GBMs), such as graphene nanoplatelets (GNP), have been explored either alone [1, 2] or in combination with other materials, generally for improvement of their native properties [3, 4]. Biocompatibility/toxicity has been thoroughly investigated, being particularly relevant when considering biomedical applications [5, 6].

The aim of this work consists on exploring the incorporation of GNP into polyurethane (PU) films. GNP were incorporated either in the bulk of the polymer, creating composites, or at the surface of the PU films, as a coating.

PU:GNP composites were produced through melt-blending by mixing the PU pellets and the GNP, in a dried powder form, in a melt compounder under high shear conditions. The nanocomposite was then extruded into an injection moulder. Regarding the GNP coatings, three different methods were explored: dip coating, where the PU substrate was dipped into a PU:GNP solution at a constant speed; spin coating, where a drop of PU:GNP solution was deposited onto the PU film surface, which was afterwards rotated at a specific speed spreading the dispersion by centrifugal force; and spraying, where an airbrush gun was used to spray a PU:GNP solution onto the PU films. Different PU:GNP concentrations in DMF or THF and PU:GNP weight ratios were used. In the case of the coatings, PU films were produced by casting after dissolution of the PU pellets in tetrahydrofuran (THF).

Materials characterization was performed by optical microscopy and by Scanning Electron Microscopy (SEM) after sputtering with Au/Pd to make samples more conductive. Several parameters were evaluated, namely the exposure of the GNP at the surface, the distribution of the GNP in the polymer, the amount of GNP found in the material as well as the influence of GNP size and oxidation degree in all these parameters.

PU:GNP composites produced by melt-blending showed a good dispersion of GNPs in the PU matrix but no significant modification of the surface, with few GNPs exposed in a planar orientation and mostly covered with polymer. On the other hand, surfaces produced by coating methods showed increased GNPs exposure at the surface, with sharp edges bursting out and only partially covered by polymer. Additionally, differences were observed when non-oxidized and oxidized GNP formulations were used, both regarding exposure and amount of GNP at the surface. In the dip coating approach, oxidized formulations led to the production of spherical structures and a more mesh-like network oppositely to what was observed when non-oxidized formulations were used. When producing the coatings through spin or spray coating, similar planar structures were found for both non-oxidized and oxidized formulations, with GNP sharp edges being exposed. Nevertheless, a smaller number of GNP was found exposed when the oxidized formulations were used.

Overall, GNP incorporation in PU films as a coating was found to improve the exposure of GNP sharp edges when in comparison with the incorporation through meltblending. Specifically, from the three coating methods explored, spin coating and spraying were found to be less time-consuming, providing more homogeneous surfaces.

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INFLUENCE OF PHYSICAL PROPERTIES OF THE TEXTILE MATERIALS IN THEIR ELETROMAGNETIC CHARACTERIZATION

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Keywords: electromagnetic characterization, dielectric properties, textiles

Wireless communication systems are made up of several electronic components, which over the years have been miniaturized and made more flexible, such as batteries, sensors and actuators. In the context of wearable systems, the antennas have been challenging because they are conventionally built on rigid substrates, hindering their efficient and comfortable integration into the garment. Considering the flexibility and dielectric intrinsic properties of textile materials, the development of textile antennas may boost wearability and enlarge the domain of applications of such wireless communication systems, aiming purposes such as tracking and navigation, mobile computing, energy harvesting and storage [1].

The knowledge of the electromagnetic properties of the materials is essential to a good design of the antenna. Many criteria should be considered, as several characteristics of the textile materials directly affect the behavior of the antenna [2]. Specific electrically-conductive textiles are available on the market and have been successfully used in the radiating components. Conventional textile fabrics have been used as substrates. However, little information can be found on the electromagnetic properties of these regular textiles. Indeed, woven, knits and nonwovens are inhomogeneous, highly porous, compressible and easily influenced by the environmental hygrometric conditions, making their electromagnetic characterization difficult [3].

The goal of the electromagnetic characterization is to measure the dielectric constant of the specimen for a specific frequency and field orientation [4]. The methods used to determine the electromagnetic properties of the materials are generally subdivided into two main categories: resonant and non-resonant methods. Each of these categories includes several procedures. The resonant methods generally give higher accuracies than non-resonant ones and do not require a complex sample preparation [5].

In this context, the main objective of this poster is to present an experimental characterization of the electromagnetic properties of some textile materials, aiming the selection of textiles well suited as dielectric substrates for the development of wearable antennas.

The Resonator-Based Experimental Technique was used. It is based on the theory of resonant methods and consists in calculate the electromagnetic parameters of the material under test, at a single frequency, by measuring the shift in frequency and the value of Q-factor of one resonator board with a microstrip patch antenna.

This technique proved to be an efficient, simple, easy and quick technique to find suitable dielectrics for textile antennas. Other advantage of this method is that the measured values are not influenced by the condition of some variables, as for example, the type of glue/adhesive sheet, the connector and the manufacturing technique of the probe, which can lead to non-repeatability of the measurements and introduce errors in the final values.

In order to understand the influence of some physical properties, such as thickness and surface roughness, on the electromagnetic behavior of the textile materials, this poster also correlates the permittivity values (measured with the Resonator-Based Experimental Technique) with the physical properties. The thickness and surface roughness of the textile fabrics were measured using the KES – Kawabata Evaluation System [6].

Also, the porosity was calculated through the density of the textile and the constituent polymer, and related with permittivity value. The superficial porosity of the faces of the textile was measured by SEM imagens using DiameterJ [7] by ImageJ software image analysis [8].

0ne observed that for all samples the side of the material with higher superficial roughness has lower permittivity value. Indeed, during the dielectric characterization when positioning the rougher face in contact with the resonator board more air is trapped on the surface of the probe, lowering the extracted value of ε_r. Furthermore, materials with high porosity value have higher permittivity values, due to the presence of air in the textile structure.

To validate the experimental characterization method, the measured permittivity values were considered for the dimensioning of wearable antennas, which performance was further tested. These antennas were designed to resonate around 2.45 GHz covering the Industrial, Scientific and Medical (ISM) band, between 2.4 and 2.45 GHz. This bandwidth also supports the WLAN (Wireless Local Area Network), Bluetooth and SRCS (Short Range Communication Systems 802.15.4) applications. The results of the antennas supported the validation of the method.

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PREPARATION AND CHARACTERIZATION OF Mn(II)-EDTA FUNCTIONALALIZED MAGNETIC NANOPARTICLES

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Manganese(II) ions combined with ethylenediamine tetraacetic acid (EDTA), as metal-based *N,O*-chelating ligands, at the surface of ferrite magnetic nanoparticles (MNPs) were prepared by a co-precipitation method [1,2]. Envisaging the application of this material towards heterogeneous catalysis it is mandatory to characterize the potential catalyst precursor. In order to get insights about the molecular composition, morphology, surface area, particle size and other relevant physical-chemical properties, spectroscopic (FTIR), X-ray (pXRD), electro probe (SEM, EDS), magnetic (VSM) and thermodynamic (TGA, BET) characterization techniques were applied.

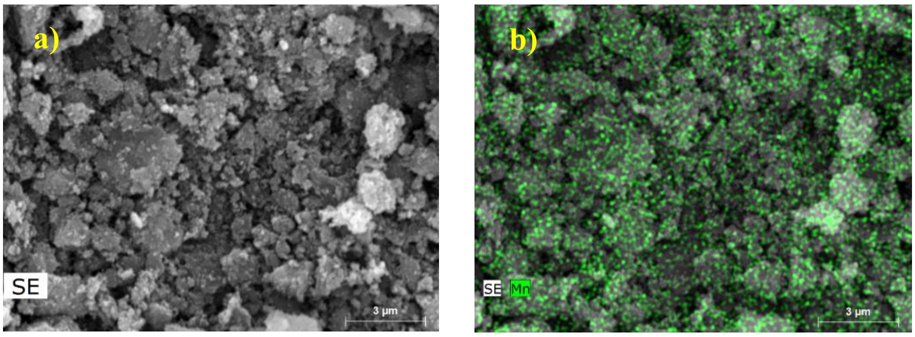

Figure 1. SEM mapping experiments on Fe_3O_4@EDTA-Mn^{2+} MNPs: a) raw micrograph; b) overlap of the raw micrograph with Mn element detection.

References

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[2] K. Azizi, M. Karimi, A. Heydari, *Tetrahedron Letters* **2015** *56*, 812–816.

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