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a word from the rector

manuel antónio assunção

university of aveiro

A university for the twenty-first century is one that promotes innovation and development based on the integration between education and research at all levels



message from the vice-rector josé fernando ferreira mendes university of aveiro

Following last year's successful first edition of research@ua, the yearly magazine that summarises the most relevant r&d results of the University of Aveiro (UA), this second edition is part of the on-going efforts to better disseminate the excellence in the research developed at the UA. In these last two years as Vice-Rector for Research and Doctoral School at UA, I became familiar with a huge number of exciting and challenging research topics developed at our university, as you are about to see in the next few pages.

Sharing the vision of the University of Aveiro, our overall mission is to contribute to the development of our region and country, as well as to the general progress of science and technology and, consequently, to a sustainable way of life for all. To this end, several strategies have been implemented in the last two years, from which I would like to highlight the creation of the Research Support Office (GAI) and the Doctoral School (EDUA). GAI was created with the main objective of promoting the

participation of our researchers The diversification of funding sources is, nowadays, a pressing need in order to promote independent and high-quality research, since national funds have been decreasing over the GAI is fully dedicated to give support to researchers; disseminate up-todate information on national and international research programmes, fellowship programs and specific provide one-to-one coaching and organization of information events. Besides, we cannot conceive a University focused on research without a direct integration of its curricula. Preparing students with courses integrating the results of research is a way to develop our own research. In order to better promote this concept UA created EDUA. This

school has the mission of coordinating the Third Cycle activities internally and externally, developing new innovative courses and increasing the admission of students.

The increasing participation in national and European networks, either at doctoral studies or projects level, the development and implementation of new technologies and the creation of new spin-offs, are some of the indicators that demonstrate that we are on the right track. For that, I would like to take the opportunity to thank all our researchers. Without their efforts, certainly, this wouldn't be possible. For the future, we will continue committed to the improvement of our r&d quality and impact, the sustainability of our personnel development and the promotion of excellence in the four strategic areas – medicine, ICT, sea and energy. I hope this small report may attract your interest and may be a driver for a future collaboration with UA!

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kissing organelles – new dynamic behaviour of peroxisomes

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Peroxisomes and mitochondria show a much closer interrelationship (the "peroxisome-mitochondria connection") than previously anticipated, which is of growing medical importance. They cooperate in the metabolism of fatty acids and reactive oxygen species, but also share components of their fission machinery. If peroxisomes - like mitochondria - also fuse in mammalian cells is a matter of debate and was not yet systematically investigated. We examined potential peroxisomal fusion and interactions in mammalian cells in an interdisciplinary approach by developing an in vivo fusion assay based on hybridoma formation by cell fusion. By combining fluorescence microscopy, live cell imaging and computational modeling we discovered that peroxisomes are engaged in transient, but vivid and long term contacts, without exchanging matrix or membrane markers. Computational analysis showed that transient peroxisomal interactions are complex, exhibit power law behavior and can potentially contribute to equilibrate peroxisome pools throughout the cell. Furthermore, we provide first evidence, that although peroxisomes and mitochondria share components of their fission machinery, mitochondrial fusion proteins (mitofusin 1, 2; OPA1) do not contribute to peroxisomal dynamics. We conclude that mammalian peroxisomes do not fuse with each other in a mechanism similar to mitochondrial fusion, but show an extensive degree of a new dynamic interaction.

OC/EC ratio observations in europe: re-thinking the approach for apportionment between primary and secondary organic carbon

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Suspended particles in the atmosphere contain a significant amount of carbonaceous matter which is commonly divided in elemental carbon (EC) and organic carbon (OC). EC is emitted directly into the atmosphere (primary EC) from incomplete burning of fossil fuels and biomass. OC may be emitted directly as particles (primary OC) or formed from gas-to-particle conversion of gaseous precursors in the atmosphere (secondary OC). Primary OC sources include combustion processes or mechanical processes that release into the atmosphere organic materials such as pollen, plant debris and soil. OC has health-relevant properties since its chemical composition includes toxic constituents and climate-relevant properties since fine OC particles are very efficient at scattering light.

The importance of the different OC sources, however, still cannot be estimated accurately because source apportion methodologies have limitations. A commonly used method for the indirect evaluation of secondary OC in aerosols is based on the minimum values of OC/EC ratios, considering that those represented samples containing exclusively primary carbonaceous aerosol from fossil fuel combustion.

A large set of carbon measurements in aerosols was used to evaluate the capability of the OC/EC minimum ratio to represent the ratio between the OC and EC fractions resulting from fossil fuel combustion. The data set covers a wide area in Europe and includes a great variety of sites. Urban background sites have shown consistent minimum ratios suggesting that it can be used as an effective tool to derive the ratio between OC and EC from fossil fuel combustion and consequently to differentiate OC from primary and secondary sources. However, our measurements undertaken in a tunnel and two road sites, in Lisbon and Madrid, strongly influenced by fresh vehicle emissions, revealed lower values for the OC/EC minimum ratio than usual measurements taken in less extreme urban environments. These results were indicative of an elevation of the OC/ EC minimum ratio with additional OC, presumably secondary, in urban background air. Therefore, the OC/EC ratios derived from the tunnel are probably more representative of road transport emissions than those derived from application of OC/EC minimum ratios taken from open air measurements in urban areas. The findings of this study may have significant implications for the development air pollutant emission inventories and may be used for more accurate simulations of the anthropogenic forcing of aerosol on climate.



women in higher education management (WHEM)

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The Women in Higher Education Management (WHEM) Network is an international research consortium. Its vision is to analyse the challenges for women in university management and to develop comparative studies about women in senior management roles. Participating countries are: Australia, Ireland, New Zealand, Portugal, South Africa, Sweden, Turkey and the United Kingdom.

The Network's first research project was published by Palgrave Macmillan in April 2011 as Gender, Power and Management: a Cross Culture Analysis of Higher Education, edited by Barbara Bagilhole and Kate White. It is the first multi-country study to examine the dynamics of men and women working together in higher education senior management teams within a broader organizational context. It is based on interviews with women and men in university senior management in the participating countries. It explores pathways into senior management, perceptions of how women and men regard each other's performance in top management jobs, and their influence on universities. It questions where women fit in university senior management, whether or not women can and do make a distinctive contribution to university decision-making, and the impact of organizational cultures on their effectiveness as managers and leaders.





modulating sperm motility

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Infertility is a growing concern in modern society, with 30% of cases being due to male factors, namely reduced sperm concentration, decreased motility and abnormal morphology. Sperm cells are highly compartmentalized, almost devoid of transcription and translation, consequently processes such as protein phosphorylation provide a key general mechanism for regulating vital cellular functions, more so than for undifferentiated cells. Reversible protein phosphorylation is the principal mechanism regulating most physiological processes in eukaryotic cells. To date, hundreds of protein kinases have been identified, but significantly fewer

phosphatases (PPs) are responsible for counteracting their action. This discrepancy can be explained, in part, by the mechanism used to control phosphatase activity, which is based on regulatory interacting proteins. This is particularly true for PP1, a major serine/threonine – PP, for which two hundred interactors (PP1 interacting proteins - PIPs) have been identified that control its activity, subcellular location and substrate specificity. For PP1, several isoforms have been described, among them PP1_y2, a testis/sperm-enriched PP1 isoform. Recent findings support our hypothesis that PP1_Y2 is involved in the regulation of sperm motility.



slow release of NO by microporous titanosilicate ETS-4

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Nitric oxide (NO) acts as an important agent in the body for expanding blood vessels (its role in Viagra and related medicines for erectile dysfunction), preventing the formation of blood clots, aiding nerve signals, and repairing wounds. NO's multipurpose role makes it an exciting prospect for new drug development, but current NO delivery



systems sometimes cause undesirable side effects. Besides good NO adsorption capacity, materials must also present an appropriate releasing kinetics, to maintain a given concentration in the surrounding milieu. Often, a slow releasing kinetics is preferred because it allows for easier and safer control of the NO concentration, for longer periods. Clearly, new materials and technologies are needed to store and target-deliver NO in biological amounts. A novel approach to design nitric oxide storage and releasing microporous agents based on very stable, zeolite-type silicates possessing framework unsaturated (e.g., pentacoordinated Ti⁴⁺) transition-metal centers has been proposed (Journal of

the American Chemical Society, 2011, vol. 133, p. 6396). This idea has been illustrated with ETS-4 [Na₉Si₁₂Ti₅O₃₈(OH)·xH₂O], a titanosilicate which displays excellent NO adsorption capacity and a slow releasing kinetics. The performance of these materials has been compared with the performance of titanosilicate ETS-10, [(Na,K)₂Si₅TiO₁₃·xH₂O], of benchmark zeolites mordenite and CaA, and of natural and pillared clays. DFT periodic calculations have shown that the presence of water in the pores of ETS-4 promotes the NO adsorption at the unsaturated (pentacoordinated) Ti4+ framework ions. The ability of ETS-4 to release biologically

relevant NO amounts was tested using the



oxyhemoglobin method, which is based on the principal reaction of oxyhemoglobin with NO to form methemoglobin and nitrate. This reaction also accounts for the inhibitory effect of hemoglobin on the biological effects of endogenous formed or exogenous applied NO.



human-related factors regulate the spatial ecology of domestic cats in sensitive areas for conservation

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Domestic cats ranging freely in natural areas are a conservation concern due to competition, predation, disease transmission or hybridization with wildcats. In order to improve our ability to design effective control policies, the factors affecting their numbers and space use in natural areas of continental Europe were investigated. We describe the patterns of cat presence, abundance and space use and analyse the associated environmental and human constraints in a well-preserved Mediterranean natural area with small scattered local farms. We failed in detecting cats in areas away from human settlements (trapping effort above 4000 trap-nights), while we captured 30 individuals near inhabited farms. We identified 130 cats, all of them in farms still in use by people (30% of 128 farms). All cats were freeranging and very wary of people. The main factor explaining the presence of cats was the presence of people, while the number of cats per farm was mostly affected by the occasional food provisioning with human refuse and the presence of people. The home ranges of eight radio tagged cats were centred at inhabited farms. Males went furthest away from the farms during the mating season (3.8 km on average, maximum 6.3 km), using inhabited farms as stepping-stones in their mating displacements (2.2 km of maximum inter-farm distance moved). In their daily movements, cats notably avoided entering in areas with high fox density. The presence, abundance and space use of cats were heavily dependent on human settlements. Any strategy aiming at reducing their impact in areas of conservation concern should aim at the presence of settlements and their spatial spread and avoid any access to human refuse. The movements of domestic cats would be limited in areas with large patches of natural vegetation providing good conditions for other carnivore mammals such as red foxes.



unveiling the structural basis for translational ambiguity tolerance in a human fungal pathogen

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The genetic code defines the rules that organisms use to synthesize their proteins from the information contained in their genes. The genes are translated into segments of three letters (triplets), meaning that DNA bases (A, C, T and G) are read three at a time during the proteins synthesis process. This translation



is done with high precision assuring that one gene corresponds to one protein only. However, in rare situations, the triplets are read ambiguously originating more than one protein from a single gene, being the alternative proteins in general toxic to cells and promote their death.

Genetic code alterations discovered during the last 40 years in bacteria, fungi, algae and ciliate organisms do not obey to the strict rules of the standard genetic code, thus posing the fascinating question of how these organisms deal with such flexibility. CESAM researchers have now demonstrated how fungi of the genus *Candida* can cope with such flexibility at the protein level. *Candida albicans* is an opportunistic fungus

that causes human infections (mainly oral and genital) known as candidiasis, which are common in immunosuppressed patients,



as the HIV and cancer patients, and elderly people. Beyond the theoretical interest of the discovery, the work reveals new facets of the biology of these fungi that could help scientists better understand the biology of infection of fungi of the genus *Candida*. The study explains how these fungi can insert different amino acids at single protein sites without disruption of protein structure. Since the environment has direct impact on genetic code fidelity this study provides deep insight on how environmental factors affect protein synthesis and on how protein structure buffers negative effects of environmental variation.

Therefore, this study reveals an unexpected flexibility of gene evolutionary mechanisms and shows how organisms survive and adapt to genetic chaos generated through genetic code ambiguity.

mineral composition of atmospheric dust in santiago island, republic of cape verde

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Aerosol sampling is being performed at Praia airport during one year (within CVDUST Project) and mineralogical composition is being studied by X-ray diffraction, TEM and Scanning electron microscopy. Structural (crystallochemical) formulas will be computed from XRD and SEM – EDAX analytical data. The identification of the main sources and origins of the particles sampled in the archipelago has been carried out in order to elucidate the role Saharan dust may play in the degradation of Cape Verde air quality.

Cape Verde is located in an area of massive dust transport from land to ocean, and is thus ideal to set up sampling devices that will enable the characterization and the quantification of the dust transported from Africa. Mineral dust produced from windblown soils and deserts is one of the largest contributors to the global aerosol loading and has strong impacts on regional and global climates, long-term climate trends as well as marine and terrestrial ecosystems. Mineralogical phases identified include various silicates and aluminosilicates, carbonates, sulphates, phosphates, oxides and hydroxides. Iron hydroxides, such as lepidocrocite and goethite, and carbonates, such as calcite and siderite, are the most discriminating phases, allowing to differentiate 3 subsets. On the contrary, silicates, such as quartz, feldspars and phyllosilicates, do not show any particular tendency, being ubiquitous and generally on small amounts. The identification of the main sources and origins of the particles sampled in the archipelago is been carried out by integrating complementary tools such as Principal Component Analysis, Positive Matrix Factorization, Chemical Mass Balance, Multilinear Regression Analysis, Air Mass Back trajectories analyses, meteorological data and particle size segregate analysis.

characterization and prediction of biomass pyrolysis products

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Environmental and social concerns, energy security and fossil fuel prices are driving increased R&D and technological interest on the utilization of renewable energy. In particular, the thermochemical conversion of biomass has been actively discussed over the past few decades as a route for producing heat, electricity and synthetic fuels in a sustainable way. Aiming to accelerate the transition from fossil fuels to renewables, a number of pilot and industrial plants were demonstrated around the world to convert biomass via pyrolysis, gasification or combustion processes.

Biomass is an organic, carbon-based solid fuel with high volatile matter content. The fuel undergoes rapid decomposition when exposed to temperatures above 250°C, forming a huge set of gas species and a non-volatile residue, called char or charcoal. Such a thermal degradation is called pyrolysis (or devolatilization) and is an important stage of fuel conversion in thermochemical processes. The characterization of this stage is of major importance in the case of biomass fuels in result of their high volatile matter content. The pyrolysis mechanism involves a great deal of physical and chemical transformations (e.g. dehydration, depolymerization) and hence the detailed description of the process is challenging. However, for engineering applications it is often sufficient to describe the ultimate yields and the properties of the pyrolytic products.

In this work, literature data on these issues has been screened and structured, constituting a guide on the general behaviour of biomass pyrolysis. The collected data covers a range of conditions with practical interest for thermochemical applications. Moreover, an empirical model to predict the distribution of pyrolytic products was proposed. The model is suitable to be integrated in comprehensive reactor models simulating pyrolysis, gasification or combustion processes, being an important tool to further develop the biomass conversion technologies.





supported ionic liquid silica nanoparticles are excellent heterogeneous catalysts for the dehydration of fructose to 5-hydroxymethylfurfural

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Diminishing fossil fuel reserves and growing concerns about global warming have fostered the development of alternative sources of energy and chemicals. Renewable biomass resources are promising alternatives for the sustainable supply of liquid fuels and chemical intermediates. The catalytic conversion of biomass is important to develop alternatives to crude oil derivatives. Among the many biomass-derived chemicals, 5-hydroxymethylfurfural (HMF) is a particularly valuable intermediate for fine chemicals, pharmaceuticals and in biofuel and polymer chemistry. Hence, acid catalyzed dehydration of fructose to HMF has received substantial attention. Homogeneous acid catalyzed processes can achieve only up to 90% fructose conversion with moderate HMF yield, and it has severe drawbacks in terms of equipment corrosion, separation and recycling; while existing heterogeneous acid catalysts can be recycled and have high HMF selectivity, but very low fructose conversion even after a very long reaction time. Consequently, more efficient catalytic systems for the selective production of HMF from fructose need to be developed.

At the University of Aveiro researchers from CICECO have recently developed supported ionic liquid nanoparticles (SILNPs) (Green Chem., 2011, 13, 340-349). The SILNPs are composed of amorphous SiO2, each sample characterized by a distinct average particle size (300 to 600 nm) that depends on the ammonia concentration employed in the synthesis by using a sol-gel method. The silica surfaces have been chemically modified with an ionic liquid via covalent attachment using a silicon alkoxide linker. The SILNPs are a new catalyst that quickly (less than 30 minutes reaction time), and efficiently (99.9% conversion), convert fructose into HMF with yields of 63% in optimized reaction conditions (130°C). These heterogeneous catalysts present improved performances over other zeolites and strong acid ion exchange

resin catalysts previously used, and were shown to be efficiently and easily recycled without any significant loss in fructose conversion and HMF yield. These new catalysts, allowing the conversion of biomass fraction into valuable products, contribute to make the biorefinery dream come true, minimizing our dependency on crude oil derivatives and advancing the world's sustainability.



direct imaging of Joule heating dynamics and temperature profiling inside a carbon nanotube interconnect

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Resistive heating is a common phenomenon when electronic components are exposed to high current densities. It leads to an accentuated waste of energy and favours electromigration, a frequent cause of circuit failure. Knowing how the building blocks of nanoscaled electronic circuits respond to such electrical stress is essential for their future use in devices. Carbon nanotubes (CNTs) have been widely touted as superior wires to connect the various components of next-generation integrated circuits. Despite almost two decades of intense effort, insight into the internal structural and thermal responses of these structures when subjected to resistive heating has been lacking. On the 9th of August 2011, in a report published by Nature Communications (doi: 10.1038/ ncomms1429), Pedro Costa from the University of Aveiro and colleagues from the National Institute for Materials Science, Japan, described how it was possible to directly image the dynamics of Joule heating and extract temperature profiles from the interior of CNTs acting as interconnects.

In general, electrical probing studies of CNTs had been performed in the absence of information concerning its internal structure, with relatively low spatial resolution and often not resolved in time. Consequently, what happened in the tubular channel during the Joule heating process remained a mystery. Working with a transmission electron microscope and an electrical probing sample holder, Costa *et al.* were able to locate the hottest points inside an electrically-heated nanotube due to the solid-to-vapour phase transitions that took place in a carbon-encapsulated semiconductor nanowire. In addition, the team also followed the migration of these hot-spots and their evolution. The sublimation fronts of the confined nanowire acted as temperature markers to understand how heat is distributed along and across the tube.

Besides CNTs, the method reported may be used to evaluate the resistive heating behaviour of other nanoscaled tubular interconnects. Eventually, it may also be envisaged as a test-bed for the study of phase transitions occurring in confined spaces such as nanometer-sized channels of porous materials.

inversion of the noisy Radon transform on SO(3) by Gabor frames and sparse recovery principles

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One of the modern methods in determining the structure of polycristalline materials is the so-called X-ray diffraction tomography. For each incidence ray one measures the diffraction pattern and from this information one desires to determine the crystallographic structure of the material. Mathematically this is done by inverting the so-called spherical Radon transform which is an ill-posed inverse problem. In the paper "Inversion of the noisy Radon transform on SO(3) by Gabor frames and sparse recovery principles", Appl. Comput. Harmon. Anal. (2011) a new method for obtaining a stable approximation of the inverse of the spherical Radon transform was established. X-ray tomography of crystallographic structures using diffraction experiments is a computationally expensive task. To give an idea of the complexity of the problem just by measuring as few as 100 incidence rays and 100 scattered rays one obtains already 10 000 measurements. The developed numerical method reduces the problem greatly by constructing new building blocks (so-called spherical Gabor frames) which allow us to use sparse recovery principles (only a few building blocks have non-zero coefficients) while maintaining a stable approximation of the inverse of the spherical Radon transform. The proposed approach is composed by basic building blocks of the coorbit theory on homogeneous spaces, Gabor frame constructions and variational principles for sparse recovery. The performance of the finally obtained iterative approximation is studied through several experiments and it was shown that this new method works well with noisy data.

Nd isotope composition of marine sediments as a tracer for iceberg provenance in the last glaciation

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OMEX core KC 024-19 was studied aiming at to assess the influence of climate changes on the origin and transport of the sediments of the Galician continental slope, in the last 40 thousand years. The sampled sediments are composed mostly of silt and clay, but also include a coarser-grained (sand-sized) fraction, corresponding essentially to foraminifera tests. Another remarkable feature is the occurrence of four depth intervals characterized by abundances greater than usual of relative large terrigenous clasts (considered as ice-rafted debris - IRD), related to melting of massive influxes of icebergs into the North Atlantic during the socalled Heinrich Events (HE). In order to obtain information on the origin of the detrital component of the sediments, 27 selected samples were submitted to a leaching procedure, to eliminate the biogenic fraction, and then analysed for Nd and Sr

isotopes by TIMS, in the Isotope Geology Laboratory of the University of Aveiro. The obtained 143Nd/144Nd and 87Sr/86Sr ratios vary from 0.512072 to 0.511604 and from 0.732273 to 0.725140, respectively. Significantly, the lowest Nd isotope ratios were obtained in samples from HE layers, namely in HE1 (~ 15 ka BP), HE2 (~ 24 ka BP) and HE4 (~ 38 ka BP). These results suggest a strong contribution of continental crustal sources significantly older than the Variscan basement for events HE 1.2 and 4. The most likely provenance of the coarse clasts deposited during these three events lie probably in NE America, where Precambrian basement occupies large areas, and the carrier icebergs should be fragments of the Laurentide Ice Sheet. This provenance is probably related to extremely cool conditions.

In contrast, the HE3 (~ 28 ka BP) layer displays Nd isotope ratios in the range of the compositions of the most common sediments in the core and, therefore, its IRD should have European source(s).



piezoelectric PLLA as a platform for tissue growth

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Imagine an implantable platform made of an intelligent material capable of thwarting bone resorption by simple electrical stimulation. PLLA, a FDA approved biomaterial, is one of the few candidates than can fulfil the challenge. Physical exercise is known to increase bone mass but the exact processes responsible for the bone growth were not untangled yet. The piezoelectric character of organic component in bone has been pointed as a possible "transducer" (converter of mechanical energy into electrical and vice versa) in bone tissue synthesis but the exact mechanisms are still unknown. The use of some piezoelectric materials to correct bone defects has demonstrated to promote a faster bone growth comparing to non piezoelectric materials. Poly (L-lactic) acid (PLLA), a semicrystalline polymer, is currently being investigated for bone regeneration purposes since it possesses a valuable combination of properties. Beyond the biocompatibility, biodegradability and adjustable physical properties, PLLA is piezoelectric. In vivo, piezo effect is expected to create charges in the surrounding area of bone and enhance regeneration processes. This research intends to shade light on how the polarization of a piezoelectric substrate influences bone growth processes.



PLLA as spin coated films, solvent casted films, nanofibers and scaffolds have been prepared. PLLA was poled by different processes: by corona poling for macroscopic polarization or locally poled at the nanoscale level by applying a DC field through a piezoresponse force microscopy (PFM) tip. The molecular orientation induced by the electrical field was checked by imaging by PFM. The electrically induced polarization of PLLA was investigated regarding its stability over time and its effect on human proteins and osteoblast-like cells. In vitro, we have shown for the first time that polarization and surface charges in PLLA have an effect on biological events occurring during bone regeneration. Polarization significantly enhances fibronectin adsorption as well as osteoblast-like cells adhesion, spreading and proliferation. We also demonstrated that in semi crystalline PLLA the polarization decay starts only after 10 days; time enough to trigger and maintain the adhesion of proteins and proliferation of cells.

asymptotics of orthogonal polynomials for a weight with a jump on [-1,+1]

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Szegö is the founder of the modern general theory of orthogonal polynomials. In particular, he was the first to prove the crucial asymptotic result for polynomials orthogonal on the interval with respect to weights that satisfy a condition that today bears his name. In the case of the classical Jacobi weights, we can derive this asymptotics (both on and away from the interval of orthogonality, as well as at its endpoints) using several identities that these orthogonal polynomials satisfy: the differential equation, the Rodrigues formula, integral representation, etc. However, in a general situation, the problem is much more difficult. Starting from the 80's, many new asymptotic results were found for various classes of weights, and the breakthrough was partially motivated by the development of the tools from potential theory and operator theory.

An important new technique for obtaining asymptotics for orthogonal polynomials in all regions of the complex plane is based on the characterization of the orthogonal polynomials by means of a Riemann– Hilbert problem for 2 _ 2 matrix-valued

functions due to Fokas, Its, and Kitaev, combined with the steepest descent method of Deift and Zhou. In a recent paper by Kuijlaars and collaborators, the complete asymptotic expansion for the orthogonal polynomials with respect to a Jacobi weight modified by a real analytic and strictly positive function was obtained. It showed that this modification does not affect essentially the local behavior of the polynomials, which has a direct implication to the study of the so-called universality property and the "clock behavior" (uniform spacing) of the zeros. A very different situation arises when the weight has a singularity on the interval of orthogonality. The case of a zero was analyzed in the work of Vanlessen, but the case of the jump singularity remained open. We consider polynomials that are orthogonal on a finite interval [_1, 1] with respect to a modified Jacobi weight with a jump at the origin. From our analysis we obtain strong uniform asymptotics of the monic orthogonal polynomials in the whole complex plane, as well as the first terms of the asymptotic expansion of the main parameters (leading coefficients

of the orthonormal polynomials and the recurrence coefficients). In particular, we prove a conjecture of A. Magnus regarding the asymptotics of the recurrence coefficients.

The main focus is on the local analysis at the origin that is made using confluent hypergeometric functions. We study the asymptotics of the Christoffel–Darboux kernel in a neighborhood of the jump, and this is the first explicit example of a non-sine reproducing kernel of a de Branges space that arises as a universality limit in the bulk of a fixed measure of orthogonality. We also show that the zeros of the orthogonal polynomials no longer exhibit the clock behavior.



promotion of students' mobility in europe: an innovative study in a virtual environment

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Virtual Learning in Higher Education (VLHE) is the name of a full semester course delivered in a virtual mobility mode. The main particularity of this course is that it was designed, developed, delivered and evaluated by six different European institutions in a fully distance mode using online synchronous and asynchronous tools. The VHLE course (6 ECTS) was delivered in the first semester of 2010/11 in English to thirty students from five different European countries (Finland,



(week 1-12) skyla Un Culturalmodels (week 10-11) (week 2-3) Aveiro University (E - Assessment strategies) University of Oviedo (UNIOVI) (Collaborative online learning) one semester course Virtual Learning in Higher Education (week 8-9) (week 4-5) Vytautas Magnus Universit (Learning Strategies) Jagiellonian University – (Information Literacy) (week 6-7) Baltic Education chnology Institute (Advanced Learning Technologies)

Lithuania, Poland, Portugal and Spain) and was divided in six different, but articulated, modules (one per institution), each one with two weeks duration.

The University of Aveiro (UA), through the Evaluation Quality Laboratory (LAQE) of the CIDTFF, participated as the responsible institution, in a collaborative way, for designing the VLHE course curricula and for planning and delivering the E-Assessment strategies module, the sixth module of the course. The majority of the teaching and learning strategies was based on the use of synchronous and

asynchronous communication strategies that were frequently used in live classes, using video conference, or in group discussions using Video-Conferencing, Skype and Google Docs. Student groups were formed in the beginning of the course, including members from the different partner countries. Students were then engaged in group and individual work and presented the results achieved in the end of each week in a live class. Given the fact that this course was developed in a research context, knowledge has been produced that hopefully may contribute to the extension of this innovative initiative (Teresevi_ien_, Volungeviciene & Dauk_ ien_, 2011).

The VLHE course was one outcome of a European Lifelong Learning project, TeaCamp, coordinated by Vytautas Magnus University (Lithuania). TeaCamp aimed to increase mobility, in a virtual environment, by facilitating the development, management and implementation of virtual mobility and research and by improving virtual mobility competences. This main objective is aligned with the European educational policy concerning the need to increase students and staff mobility as a key element for the European Area of Higher Education. Further information can be found in the TeaCamp website: http://www.teacamp.eu/

CO₂ emission allowances and other fuel markets interaction

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This empirical work examines interactions between carbon, electricity and fossil fuel (coal, oil and natural gas; primary energy prices used in electricity generation) returns. Impacts of emission trading are studied with the Vector Error Autoregressive Correction Model (VECM) approach, for 5 endogenous variables, using monthly data from October 2005 to October 2009, throughout Europe (Germany, France and Nordic countries), by taking into account their heterogeneity. This enabled us to reveal the difference in responses to carbon constraints in the electricity generation sector and to evaluate the efficiency of the EU ETS. Results reveal that nuclear power generation could limit increases in prices of electricity and that the effect of carbon



depends on the energy mix and electricity deregulation stage of the country under analysis. It seems that in the European Energy Exchange (EEX) more carbon coercion was undergone and innovations in carbon are stronger in electricity prices. In sum, carbon constraints on the cost of coal and electricity production depend on the country analyzed, which addresses an answer to the impact of the recently created European Union Emission Trading System (EU ETS). Producers in countries using predominantly fossil fuels, big carbon emitters, had undergone more carbon coercion and thus were more likely to include the price of emission permits in their electricity generation and cost functions (EEX). We also found that electricity is the major source of randomness that drives the carbon market for EEX, and vice versa, being the major source of randomness for carbon in France, but not vice versa in this case. In contrast, in the Nord Pool market, the major sources of randomness for carbon are electricity, gas and oil (much lower for coal), gas and oil being used almost in the same percentage in the Nordic countries to generate electricity.

Throughout the period analyzed, the efficiency of the European market for emission allowances had not been able to compel electricity producers to reduce their emissions and invest in cleaner technologies, despite being a good step towards achieving the objectives of the Kyoto Protocol. Desired effects to be produced also depend on politics pursued in distributing allowances.



mobility between heterogeneous networks

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Ubiquitous Internet access is one of the main challenges for the telecommunications industry in the next decade. The number of users accessing the Internet is growing exponentially and the network access paradigm of "always best connected, anytime, anywhere" is a central requirement for the so-called Next Generation Mobile Networks (NGMN). WiMAX, together with 3GPP LTE, was recently recognized by ITU as one of the compliant access technologies for 4G. Nevertheless, WiMAX is not yet fully prepared for next generation environments, mainly due to the lack of end-to-end QoS procedures to support real-time multimedia services delivery. Furthermore, besides the 4G compliant WiMAX and 3GPP LTE radio access technologies, 3GPP UMTS/HSPA and Wi-Fi will also have a significant impact in the mobile communications during the next decade. Therefore, it is fundamental to enable the coexistence of several radio access technologies, thereby providing mobile users with seamless mobility. In this work and related projects, it is



proposed a seamless mobility architecture with QoS support in heterogeneous wireless access environments. The proposed architecture integrates an extended version of IEEE 802.21 framework with QoS support, as well as an advanced mobility manager integrated with the Mobile IP (MIP) mobility management protocol. It is also proposed an extension to the handover decisionmaking processes in heterogeneous access environments through the integration of context information from both the network elements and the end-user. Performance tests are developed in a real testbed to validate the proposed optimizations in an inter-technology handover scenario involving WIMAX, WI-FI and 3GPP UMTS/HSPA. This research work has a strong impact in industry, and simpler versions of the developed architecture are being developed towards products, related with heterogeneous wireless access networks coexistence: a connectivity management product ("MyConnect") and a seamless mobility management pre-product ("MyMove").

SARDANA – first time demo of 1000 clients on a single reconfigurable passive optical access network

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FTTH is nowadays a must have in most developed and even in developing countries. Investments are being made allover to try and minimize the "digital divide". For that, several are the problems being raised among all players in this ecosystem: the users, the operators, the service content providers, the regulators and any newcomer. Portugal, following many countries, is leading the number of homes with fiber already passed to it. It is still gathering traction on the number of connected users, by now only early takers, but fast moving to a massive access to ultra high bandwidth services. Besides the changes this will bring to the way people act, this will effectively open a set of new opportunities (new services, new ways of working, etc).

However, despite the fact that this is a high interest and investment field, the number of barriers that prevents this business of being a full success is high, namely the full availability at a sustainable cost, the deployment strategies, the competition, and others. Contributing to these high level problems the SARDANA project promoted several state of the art technologies which enable to overcome most of these limitations. The project observed concepts like "colourless ONUs", which allow the same set top box to be used agnostically to the provider assigned band, allowing with this, mobility within operators and openness (a regulatory trend). Also, with the ring architecture inserted in the PON, failures can be worked out very fast minimizing the down time, therefore reducing outage and service prevention, very critical for high priority services or situations. By developing intelligent self-sustained harvesters and low power electro optic mechanisms, the healing and redefinition of the network becomes automatic and self-regenerative, increasing quality of service and flexibility when changing the network. Also, remote amplification, allows full passiveness of the outer plant, and still cover remote areas (100km distant) as well as 1000+ subscribers from a single active central office. This is a big step into reducing the digital divide and allowing seamless evolution of the networks. SARDANA has contributed to standards, won an award, produced more than 100 publications and pushed the directions of deployments (e.g the ARENA Italian project) and future networks.

zirconia based phosphors

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Nowadays, huge efforts are being put in technologies which promote energy savings namely in the solid state lighting (SSL) area from which economic benefits are expected. Such advances require key science challenges, including the development of innovative functional materials, new device design and progresses on light extraction. GaN-based wide band-gap semiconductors are among the most used LED-based light sources. However, the low efficiency and droop of the green component of such LEDs limits the performance of red-greenblue (RGB) based SSL systems, especially when white light sources are envisaged. A promising alternative approach to the production of white light for replacement of conventional light sources is phosphor converted white emission by a photoluminescence mechanism. These devices operate by pumping yellow phosphors (YAG:Ce3+) with blue GaN

- based LEDs. In order to enhance the color rendering index (CRI), new phosphor materials must be exploited. In this framework, due to their outstanding optical, chemical and mechanical properties, zirconia-based hosts appear as major candidates for replacing YAG:Ce3+, Zirconia exhibits a wide band gap and allows the incorporation of active lanthanide dopants. Our results demonstrate that red, green and white emission can be obtained by optically pumping Tb3+, Eu3+ (or Pr3+) and Dy3+ doped zirconia, respectively. These phosphors were obtained by two different routes, namely the laser floating zone (LFZ) for monocrystalline fibres and selfcombustion for nanometric powders. Both approaches resulted in room temperature bright visible light emission, as can be seen in the images. The white emission obtained in ZrO2:Dy3+ is highlighted due to its technological importance.



international stock market indices comovements: a new look

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It is of considerable interest to investors and financial market regulators to examine how vulnerable stock markets are to different financial shocks. We provide additional evidence on breaks in linkages between crisis capital markets. The usefulness of wavelet analysis to financial contagion and comovement is illustrated. considering that international investors distinguish between short and long run relations. Continuous wavelet and crosswavelet analysis have the ability to analyze transient dynamics for single time series, or for their association, allowing, thus, for a multivariate (bivariate) analysis. This study accounts for the time-varying pattern of price shock transmission, exploring stock market linkages using continuous time wavelet methodology. In order to sustain and improve previous results regarding correlation analysis between stock market indices, namely FTSE100, DJIA30, Nikkei225 and Bovespa, we extend here such analysis using the Coherence Morlet Wavelet. Results indicate that the relation among indices was strong but not homogeneous across scales, that local phenomenon's are more felt than others in these markets and that there seems to be no quick transmission through markets around the world, but yes a significant time delay. Innovations in the US and UK stock markets are not rapidly transmitted to other markets, which may induce arbitrage opportunities. Moreover, business cycle periods, corresponding to historical financial crisis periods, were identified, where the series show higher coherence, but mostly at low frequencies, favouring the contagion hypothesis during



these periods. Also, geographically and economically closer countries exhibit higher levels of market linkages, as suggested by previous authors, and the Japanese market, in general, presents a low comovement with the other countries considered. Finally, the importance of historical transmissions has decreased in the last decade, with the exception given for the period 2007–2009.

sampling in engineering and mathematics

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In 1900, David Hilbert put forth a collection of problems that he believed could shape the course of mathematics in the twentieth century. In his famous address to the International Congress of Mathematicians of 1900 he mentioned ten of those problems. The expanded version of his speech, published soon after the congress, contained 23 problems. Hilbert's notebook mentioned yet another one, related to the question of "simplicity of a theorem" and the role of "equivalences":

"Criteria of simplicity, or proof of the greatest simplicity of certain proofs. Develop a theory

of the method of proof in mathematics in general. Under a given set of conditions there can be but one simplest proof. Quite generally, if there are two proofs for a theorem, you must keep going until you have derived each from the other, or until it becomes quite evident what variant conditions (and aids) have been used in the two proofs. Given two routes, it is not right to take either of these two or to look for a third; it is necessary to investigate the area lying between the two routes ... " Part of the interest in equivalence groupings is due to the information that they reveal about the area lying between the equivalent propositions. At IEETA, a team of senior researchers from 5 countries, partially supported by the FCT, has been investigating sampling (AMS subject classification 94A20), interpolation and Fourier analysis. The goal is to clarify the connection between these topics, which are of interest to both mathematicians and engineers, and lie at the heart of mathematical analysis. Simultaneously, the team has uncovered new results in the history of the subject. The results (more than 180 pages in 2011) have been published in mathematical and engineering journals, including The Journal of Fourier Analysis and Applications and Notices of the AMS, the most widely read journal in mathematics, contributing a great deal to the visibility of the e_ort.



why does mercury spins as it does?

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The rotation of Mercury is presently trapped in a 3/2 spin-orbit resonance. This means that the planet rotates three times about its spin axis for every two orbits about the Sun. However, recent observations with the Messenger spacecraft have shown that it was not always so. An international team of astronomers, including Alexandre Correia from the Physics Department, University of Aveiro, found strong evidence that the planet once rotated synchronously with the Sun (as the Moon does with the Earth). The team also explained how the present 3/2 configuration could be obtained due to impacts with large asteroids, starting from a retrograde rotation.

Using computer models that simulate the long-term evolution of Mercury's rotation, the team started the simulations by assuming that Mercury initially had a retrogade rotation (east-to-west) in the past instead of a prograde one (west-toeast). Current planet formation models



suggest that the initial spin of terrestrial planets in the Solar System could have been either prograde or retrograde - with equal probability - so making such an assumption is not outlandish. In this situation, it was shown that Mercury evolves to the synchronous resonance naturally. Moreover, in contrast to previous studies, the new model can make real predictions about the density and distribution of impact craters on the surface of Mercury. For a synchronous orbit, for example, the model implies that there should be more craters on the dark side of Mercury - that is, the side that does not face the Sun. This is exactly what astronomers observe today when they analyze Mercury's craters data from Messenger.

The calculations also suggest that a large asteroid impact may have disrupted this initial synchronous rotation. A giant impact like the one that formed the Caloris Basin unlocks the spin from the synchronous resonance and the planet subsequently evolves into the present 3/2 observed state. Researchers will now look for other evidence of the initial synchronous rotation, such as different thicknesses in the lithosphere (the rigid, outermost shell of a rocky planet) on the light and dark sides of Mercury. The Messenger probe, currently in Mercury's orbit, will hopefully provide further insights.



absent words in genomic sequences

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Genomes can be abstracted as a sequence of four letters representing the nucleotides. The convenience of this simplification goes beyond representation, to exploring properties of finite-sized strings over finite alphabets in genome analysis. One such property is the existence of a set of absent words. Absent words in genomic sequences are surprising because of the typically large size of the sequence (approximately 6 billion letters in the haploid human genome), the small alphabet size (4 letters), and the small size of the shortest absent words (11 letters in the reference human genome). The set of all words not present in a genome is of limited biological interest. Hence, we have introduced a new class of absent words designated minimal absent words. By definition, minimal absent words have at least three letters and the removal of their left- or rightmost character uncovers a word that is present in the sequence. For illustration, consider sequence ACGGCGGCTTC. Its set of minimal absent words is {ACT, CGC,CTC,GGG,TCG,TCT,TTT,ACGGC T,GCGGCG}. Consider word ACT from this set. This word does not occur in the sequence. However, words AC and CT do occur. Hence, ACT is a minimal absent word of the sequence above. The core of a minimal absent word, that is, the word that remains after removing the left- and rightmost characters (for example, CGGC in the minimal absent word ACGGCT), is



a maximal exact repeat. Maximal exact repeats are key for seeding alignment of sequencing reads from massively parallel methodologies in genome assembly, and as anchor points in comparisons of closely related genomes.

Minimal absent words have been ubiquitously computed in genomes of organisms from all domains of life. The figure displays the number of minimal absent words (MAWs) as a function of the length of the minimal absent word in the genomes of 22 organisms. These include one archaeota (Mi), thirteen bacteria (Ba, Bs, Ec, Hi, Hp, Lc, Ll, Mg, Sa, MRSa, MSSa, Sp, Xc), and eight case-study eukaryotes (Sc, At, Ce, Dm, Gg, Mm, Pt, Hs). Though here not displayed, these genomes contain many more and much larger minimal absent words. We have investigated if the hypothesis of mutational biases (namely, the hypermutability of CpGs) as an explanation for the absence of the shortest absent words in vertebrates is valid for larger minimal absent words and in

other organisms, but found no evidence supporting it. We have also investigated the hypothesis of the inheritance of minimal absent words through common ancestry, in addition to lineage specific inheritance, and found this inheritance may be exclusive to vertebrates. As minimal absent words are intrinsically related to maximal exact repeats in the genome and not bound to protein-coding regions, they may be useful for inferring de novo genomic homology and uncovering new information on the evolution of genomes. Such strategy would overcome the failure to detect homology when there is considerable sequence divergence by current genomic homology inference methods, as well as, their typical disregard for the non-protein-coding regions of the genome. This might prove particularly useful in genomes with high repeat content, such as the human genome, where more than half of the sequence remains 'dark matter', with only _1.5% exons and _44% repetitive sequences presently annotated.

material and the flow of electrons between different materials. In bulk silicon, this is commonly achieved by introducing dopants in the material, but this method has limited success in small silicon nanoparticles.

Since small nanoparticles have a large surface-to-volume ratio, an alternative is to use surface manipulation as a means to modify the electronic properties of the nanoparticles. We have proposed that organic molecules in contact with the nanoparticles can be used to extract electrons from them. For example, first-principles calculations show that the adsorption of $F_4 - TCNQ$ (7.7.8.8 - Tetracvano - 2.3.5.6 tetrafluoroquinodimethane), an organic molecule with an extraordinarily high affinity for electrons, on the surface of silicon nanocrystals, leads to the formation of a hybrid electronic state shared by both moieties and results in the displacement of the electron density towards the adsorbed molecule. With a coverage ratio of just three F₄ – TCNQ molecules per silicon nanocrystal, it is possible to extract one electron charge from 2 nm nanocrystals. Thus, F₄ – TCNQ can be used as a surface dopant alone, or in conjunction with other p-type dopants, to increase the hole density in the proximity of the surface. This opens up new ways to control the properties of the nanoparticles from the exterior.



designing nanoparticles for electronics

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Researchers from the I3N – Institute for Nanostructures, Nanomodelling and Nanofabrication have recently proposed alternative ways to tweak the properties of silicon nanoparticles (DOI: 10.1103/PhysRevB.84.125437). These particles, of the scale of a few nanometers, have been object of intense study in recent years and regarded as a possible material for future solar cell technology.

Solar cells however, as many other electronic devices, are based on p-n junctions, sharp junctions between a material that is rich in electrons and a material that is poor in electrons, or in other words, that is rich in holes. Thus, solid state electronics and optoelectronics rely on the ability to control the excess or deficiency of electrons in a

distributed broadband wireless systems based on optical infrastructure atílio gameiro

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There are currently in the wireless arena considerable researches aiming at what is commonly called 4G systems that are spurred by interdependent technical and economical / deployment trends. Such 4G systems should fulfil several goals, among which: provision of true broadband , increase of the system level capacity; fairness access and power efficiency. It is more or less consensual that to achieve targets outlined for systems beyond IMT-2000, will require the use of MIMO (Multiple-Input Multiple-Output) technology based on multiple antennas at the transceivers to exploit the scattering properties of the wireless medium. Unfortunately due to the physical limitations in the size of the transceivers, the number of antenna elements cannot be large and furthermore the spacing between them is limited. At IT-Aveiro and within the ICT FUTON project a novel architecture has been proposed which is based on a Distributed Antenna System (DAS) supported by an optical infrastructure. The mobiles communicate simultaneously with several antenna units, with the broadband and low loss characteristics of the optical fibre ensuring perfect cooperation between them. This allows the antennas to be treated as physically distributed antennas of one composite base station and achieve distributed MIMO.

The architecture proposed brings several advantages both in terms of system performance as well as CAPEX/OPEX. In addition to the cooperative MIMO, it allows namely, the Transparent support of legacy (2G, 3G) and future high capacity RATs (4G) over a single infrastructure, facilitate the implementation of Cooperative MIMO and integration of macro and small cells. The project has developed several solutions towards the concept and has shown the technical feasibility of fibre supported cooperative MIMO, by developing an experimental testbed demonstrating of cooperation mechanisms for LTE-Advanced bit rates employing two remote antenna units connected to the central unit though optical fiber with several pedestrian users. This research is expected to have impact on the industry, with these concepts and integration of the optical and wireless technologies being strongly pushed by the major Chinese manufacturers.



allergic asthma on the breath: metabolomics brings diagnosis a step closer

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Allergic asthma represents an important public health issue with significant growth over the years, especially in the paediatric population. Currently, diagnosis is based upon symptoms and in the measurement of non-specific and broad biomarkers. The present study is based on the analysis of exhaled breath (EB), a non-invasive, easily performed and rapid sampling approach. EB is a rich source of data with potential to provide valuable information about respiratory

and systemic diseases that can lead to a deeper knowledge of human health status. Studies have been performed in our group concerning the optimization of several parameters of EB sampling. EB metabolites were analyzed by comprehensive twodimensional gas chromatography-time of flight mass spectrometry, which leads to the identification of several hundred compounds pertaining to different chemical families. Multivariate analysis plays an important role in understanding which metabolites are characteristic of asthmatic children exhaled breath and a "breath-print" of 134 volatile compounds was identified that allowed the distinction between allergic asthmatic and control children. This data set comprises compounds possibly linked to oxidative stress, inflammation processes or other cellular processes that may characterize asthma. A pattern of six compounds pertaining to the alkanes characterized the asthmatic population and on to otherwise, a set of aldehydes characterized the control population. Nevertheless, for clinical purposes, and having in mind that molecular diagnosis is thought to be the next step in clinical practice, this pattern formed by the six alkanes and the aldehydes was tested and the results accentuate the possibility of EB analysis, not only in a metabolomic point-of-view for allergic asthma knowledge, but also in clinical applicability as a possible add-in to the standard tests performed actually. The uprising issue of personalized medicine led to the monitorization of a child that had never taken an asthma drug (naive). The results of this study provided a novel methodological approach to characterize allergic asthma as a function of its metabolomic patterns, which will open new strategies to early diagnosis, therapy monitoring, and understanding the asthma pathogenesis that affects millions around the world.



organic synthesis. new products with potential applications

organic chemistry research group

department of chemistry & QOPNA, university of aveiro



A) Structural features and amphiphilic properties are required for a new porphyrin derivative to be considered as a photosensitizer (PS) in photodynamic therapy (PDT). In such way chlorins and bacteriochlorins, as well as certain cationic and glycoconjugate derivatives, have been targets for several research groups. We have been able to establish that certain porphyrin macrocycles can act as dienophiles or dipolarophiles in cycloaddition reactions; in such way novel chlorins and bacteriochlorins and some glycoconjugates and novel cationic derivatives can be obtained. In collaboration with other groups the new products have been assessed as photosensitizing agents in PDT or in the photoinactivation of microorganisms. In particular, the action against antibiotic resistant bacteria, mainly the Gram (-) ones, is of great significance. It is also possible to photoinactivate microorganisms present in water samples, including sewage ones. Such potential applications have been patented. B) Inflammatory processes are complex physiological responses, which involve an increase in vascular permeability as well as overproduction of reactive oxygen and nitrogen species. If these reactive species overcome host defense systems, damage in inflammatory sites can occur, contributing to chronic diseases. In order to control these diseases, anti-inflammatory substances possessing antioxidant properties need to be used. Polyphenols have important biological properties. The similarity of 2-styrylchromones with flavones and their known biological activities led us to develop new synthetic methods for this type of compounds and to design novel



CH.

molecules presenting antioxidant, antiinflammatory, and anti-norovirus activities. 2-Styrylchromones were starting materials, throughout cross-coupling reactions, for the development of a novel group of polyhydroxy-2,3-diarylxanthones, which already demonstrated potent antioxidant activities. Biological applications of these compounds gave rise to a European patent application.



 $R^1, R^2, R^3, R^4, R^5, R^6 = H \text{ or OH}$

mass spectrometry approaches to study breast cancer

mass spectrometry group: luisa helguero, zita cotrim, rui vitorino, ma. luisa doria, rita ferreira, pedro domingues, rosário domingues, francisco amado

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Breast cancer is the most common cancer in women and represents a major public health problem. Although early detection and recent advances in treatment have reduced the mortality rates, most breast cancers develop resistance to therapy. Therefore, it is necessary to identify novel therapeutic targets as well as markers of disease progression and resistance to therapy. Our lab is currently focused on two lines of research:

1) Extracellular matrix and estrogen signalling: Most breast cancers express estrogen receptors (ER) and depend on estrogen to grow. These cancers are treated with endocrine therapy, by blocking estrogen synthesis and ER action with antagonists. ERs are ligand activated transcription factors, subjected to a myriad of posttranslational modifications (PTMs) including phosphorylation. Such modifications alter ER affinity for a ligand and ER transcriptional activity. In addition, hyperactive kinase pathways which target ER are often associated to endocrine resistance. Our aim is to identify modulators of such signalling pathways in the extracellular matrix (ECM) of endocrine sensitive and resistant tumours and associate their expression to ER PTMs. For this purpose, extracellular matrix proteins were extracted, separated by

SDS-PAGE and identified by MALDI-TOF/ MS. In parallel, ER from the same tumours were purified using an E2 affinity column and PTMs will be identified by LC-MS/ MS. Results from this work will allow identification of proteins with prospective use as markers and/or therapeutic target in endocrine resistant tumours. 2) The role of lipids in breast cancer has been largely understudied. Besides their contribution to the cell membrane mass, lipids regulate membrane fluidity, are an energy source and have roles in cell signalling; all processes altered in malignant progression. We used a lipidomic approach in which phospholipids were separated by thin layer chromatography and analyzed by ESI-MS/MS. Differences in the spectra of sphingomyelins and phosphoinositides - two PLs with roles in regulation of cell survival and motility - were found between non malignant and breast cancer cells with different degrees of aggressiveness. Presently, we are extending these studies to breast tumours with the aim to identify prospective biomarkers of disease progression.



an alternative to kinematic hardening in classical plasticity

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- ³ institut national polytechnique de grenoble, france

In metal forming, numerical simulations are very useful to optimize processes, and thereby, decrease development time and cost. Accurate results are achievable if sufficient consideration is paid to the choice of the numerical parameters, including type of mesh, boundary conditions and material constitutive behavior. In plasticity, multi-scale modeling has been instrumental for understanding the relationship between macroscopic properties and microstructural features at different scales and has been successfully applied for material design. Philosophically, multi-scale is a very comprehensive and interpretive approach to constitutive modeling. However, in many instances, it does not address very well the practical manufacturing needs, e.g., in the sheet forming industry when simple, yet accurate, material models with timeefficient implementations in commercial finite element (FE) codes are required. This is a domain where continuum descriptions are still very powerful. Plasticity in metals is a phenomenon that is mainly controlled by dislocation glide on slip systems occupying weak or strong preferred orientations. The fields of dislocations dynamics and crystal plasticity have been very active over many decades to qualitatively and quantitatively understand the numerous mechanisms occurring during plastic deformation. The effects of crystal plasticity have been roughly captured at the continuum level by the introduction of non-quadratic yield functions/plastic potentials. These functions have been employed successfully in a number of examples where loading is nearly proportional. However, this is no longer the case when a material is subjected to cross-loading or stress reversal.

In this work, an approach is proposed for the description of the plastic behavior of materials subjected to multiple or continuous strain path changes. In particular, although it is not formulated with a kinematic hardening rule, it provides a

reasonable description of the Bauschinger effect when loading is reversed. This description of anisotropic hardening is based on homogeneous yield functions/ plastic potentials combining a stable, isotropic hardening-type, component and a fluctuating component. The latter captures, in average, the effect of dislocation interactions during strain path changes. For monotonic loading, this approach is identical to isotropic hardening, with an expanding isotropic or anisotropic yield surface around the active stress state. The capability of this constitutive description is illustrated with applications on a number of materials, namely, low carbon, dual phase and ferritic stainless steel samples.



integrated biomimetic carbon nanotube composites for *in vivo* systems

manoj kumar singh¹, josé gracio¹, philip leduc², paula gonçalves³, paula marques¹, gil gonçalves¹, filipa marques³, virgília silva³, fernando capela silva⁴, joana reis⁴, jose potes⁴, antónio sousa¹

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- 4 university of evora



As interest in using carbon nanotubes for developing biologically compatible systems continues to grow, biological inspiration is stimulating new directions for in vivo approaches. The ability to integrate nanotechnology-based systems in the body will provide greater successes if the implanted material is made to mimic elements of the biological milieu especially through tuning physical and chemical characteristics. In this work, is demonstrated the highly successful capacity for in vivo implantation of a new carbon nanotubebased composite that is, itself, integrated with a hydroxyapatite-polymethyl methacrylate to create a nanocomposite. The success of this approach is grounded in finely tailoring the physical and chemical properties of this composite for the critical demands of biological integration. This is accomplished through controlling the surface modification scheme, which affects the interactions between carbon nanotubes and the hydroxyapatite-polymethyl methacrylate. Furthermore, carefully examination of cellular response with respect to adhesion and proliferation to examine in vitro compatibility



capacity is carried out. The results indicate that this new composite accelerates cell maturation through providing a mechanically competent bone matrix; this likely facilitates osteointegration *in vivo*. These results will have potential applications in a diversity of areas including carbon nanotube, regeneration, chemistry, and engineering research.





Celebrating the scientific and research achievements of UA is what "research day" is all about. Over the previous years, great progress has been made as far as research output at the UA is concerned. On the university's Research Day some of the outstanding research outcomes achieved were presented and shared by postgrad students, researchers and professors. The University's researchers are actively engaged in a wide variety of cutting-edge investigation with high impact in society, outreaching the objectives of the European Research Area. Most of these studies were presented in the form of a poster or a short lecture.

wednesday 8th june 2011

EARCH DAY



A panel of specialists in several scientific areas highlighted the scientific rigor, the theoretical reasoning, the adequacy of the format, the obtained results and the transdisciplinarity and originality of seven out of 113 projects presented at "Research day". Four honorific mentions were also assigned. Throughout the day, about 900 faculty, researchers and PhD students from the four associate laboratories and 14 research units of the University of Aveiro presented their outstanding R&D results.



IN REVIEW



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PhD and master theses

PhD theses in 2011 per area

 s_{0} , mathematics s_{0} ,

others: biochemistry; materials science and engineering; environmental applied sciences; design; physical engineering; informatics engineering; chemistry engineering; industrial management; literature; environmental sciences and engineering; culture; economy; civil engineering; psychology; telecommunications; biomedical sciences; communication sciences and technologies; accounting; biomedical engineering; art studies; linguistics; tourism. master theses in 2011 per area



others: physical engineering; public administration and management; didactics; gerontology; design; forensic psychology; psychology; visual arts teaching – 3rd cycle of basic schooling and secondary schooling; biochemistry; editorial studies; chemistry; molecular biomedicine; materials engineering; specialised translation; tourism management and planning; economics; microbiology; music; sustainable energy systems; environmental engineering; mathematics and applications; pharmaceutical medicine; speech and hearing sciences; languages, literatures and cultures; meteorology and physical oceanography; regional and urban planning; eeological engineering; languages and business relations; accounting and public administration; ecology, biodiversity and ecosystem management; governance, competitiveness and public policies; mathematics teacher education – 3rd cycle of basic schooling and secondary schooling; physics; political science; toxicology and ecos sciences; geomaterials and devices; ceramices and glass engineering; coastal and ocean sciences; geomaterials and geological resources; marine biology; analytical chemistry and quality assurance; materials derived of renewable resources; molecular and cell biology; physics and chemistry teacher education – 3rd cycle of basic schooling.

SCI papers

top 10 subject areas for papers published in 2011

	record count	% of 1110
chemistry	250	22,52%
materials science	169	15,23%
engineering	148	13,33%
physics	146	13,15%
environmental sciences ecology	126	11,35%
mathematics	65	5,86%
biochemistry molecular biology	44	3,96%
toxicology	42	3,78%
optics	41	3,69%
computer science	33	2,97%

published papers @ua



top 10 cited papers

	[2007 · 2011]
Dorogovtsev, S.N.; Goltsev, A.V.; & Mendes, J.F.F. (2008). Critical phenomena in complex networks. <i>Reviews of Modern Physics</i> , 80: 1275-1335	254
Carlos, L.D.; Ferreira, R.A.S.; Bermudez, V.Z.; & Ribeiro, S.J.L. (2009). Lanthanide-Containing Light-Emitting Organic-Inorganic Hybrids: A Bet on the Future. <i>Advanced Materials</i> , 21: 509-534	182
Butler, G.; Rasmussen, M.D.; Lin, M.F.; Santos, M.A.S.; Sakthikumar, S.; Munro, C.A.; Rheinbay, E.; Grabherr, M.; Forche, A.; Reedy, J.L.; Agrafioti, I.; Arnaud, M.B.; Bates, S.; Brown, A.J.P.; Brunke, S.; Costanzo, M.C.; Fitzpatrick, D.A.; de Groot, P.W.J.; Harris, D.; Hoyer, L.L.; Hube, B.; Klis, F.M.; Kodira, C.; Lennard, N.; Logue, M.E.; Martin, R.; Neiman, A.M.; Nikolaou, E.; Quail, M.A.; Quinn, J.; Santos, M.C.; Schmitzberger, F.F.; Sherlock, G.; Shah, P.; Silverstein, K.A.T.; Skrzypek, M.S.; Soll, D.; Staggs, R.; Stansfield, I.; Stumpf, M.P.H.; Sudbery, P.E.; Srikantha, T.; Zeng, Q.; Berman, J.; Berriman, M.; Heitman, J.; Gow, N.A.R.; Lorenz, M.C.; Birren, B.W.; Kellis, M.; & Cuomo, C.A. (2009). <i>Evolution of pathogenicity and sexual reproduction in eight Candida genomes</i> . Nature. 459: 657-662	130
Santos, L.M.N.B.F.; Lopes, J.N.C.; Coutinho, J.A.P.; Esperanca, J.M.S.S.; Gomes, L.R.; Marrucho, I.M.; & Rebelo, L.P.N. (2007). Ionic liquids: First direct determination of their cohesive energy. <i>Journal of the American Chemical Society</i> , 129: 284-285	128
Martianov, I.; Ramadass, A.; Barros, A.S.; Chow, N.; & Akoulitchev, A. (2007). Repression of the human dihydrofolate reductase gene by a non-coding interfering transcript. <i>Nature</i> , 445: 666-670	121
Gardas, R.L.; Freire, M.G.; Carvalho, P.J.; Marrucho, I.M.; Fonseca, I.M.A.; Ferreira, A.G.M.; & Coutinho, J.A.P. (2007). High-pressure densities and derived thermodynamic properties of imidazolium-based ionic liquids. <i>Journal of Chemical & Engineering Data</i> , 52: 80-88	110
Gandini, A. (2008). Polymers from Renewable Resources: A Challenge for the Future of Macromolecular Materials. Macromolecules, 41: 9491-9504	109
Pinna, N.; & Niederberger, M. (2008). Surfactant-free nonaqueous synthesis of metal oxide nanostructures. <i>Angewandte Chemie International Edition</i> , 47: 5292-53043	108
Harbuzaru, B.V.; Corma, A.; Rey, F.; Atienzar, P.; Jorda, J.L.; Garcia, H.; Ananias, D.; Carlos, L.D.; & Rocha, J. (2008). Metal-organic nanoporous structures with anisotropic photoluminescence and magnetic properties and their use as sensors. <i>Angewandte Chemie International Edition</i> , 47: 1080-1083	107
Freire, M.G.; Carvalho, P.J.; Fernandes, A.M.; Marrucho, I.M.; Queimada, A.J.; & Coutinho, J.A.P. (2007). Surface tensions of imidazolium based ionic liquids: Anion, cation, temperature and water effect. <i>Journal of Colloid and Interface Science</i> , 314: 621-630	104

international projects

EU – funded projects started in 2011

seventh framework programme – projects coordinated by UA	acronym	project coordinator
Integrated water resources and coastal zone management in European lagoons in the context of	LAGOONS	Ana Lillebo
climate change		
Nanoeletromechnical motion in functional materials (ITN)	NANOMOTION	Andrei Kholkine
seventh framework programme	acronym	local coordinator
Dopant-surface interactions in silicon nanoclusters	SiNanoTune	José Coutinho
Smart intelligent aircraft structures	SARISTU	Mikhail Zheludkevich
Technology platform for point-of-care diagnostics for tropical diseases – EU	PodiTrodi-EU	Andrei Kholkine
Robustness by autonomous competence enhancement	RACE	Luís Seabra Lopes
Producing a shared vision on how to harness research & development for sustainable development	Vision RD4SD	Carlos Borrego
Enhancing scanning lon-selective electrode technique	SISET	Mikhail Zheludkevich
Enhancing the capacities of the ELIRI Research Institute in applied research to enable the integration	MOLD-NANONET	Nikolai Sobolev
of Moldava in the European Research Area on the basis of scientific excellence		
research fund for coal and steel	acronym	local coordinator
Modelling of atmospheric corrosion of steel protected by aluminium based alloys, applied by hot	ATCORAS	Mikhail Zheludkevich
dip processing		
Durability of adhesively bonded surfaces finished galvanized steels in corrosive environments	DURADH	Mikhail Zheludkevich
Fire design of steel members with welded to hot-rolled class 4 cross-section	FIDESC4	Paulo Vila Real
Membrane action in fire design of composite slab with solid and cellular steel beams	MACS+	Paulo Vila Real
interreg iv	acronym	local coordinator
Rede de cooperação e transferência para a aplicação de materiais de alto valor acrescentado com	CarbonInspired	Joana Madaleno
base em nanoparticulas carbonosas no sector automóvel e da construção"		
Red International en análisis de ciclo de vida y ecodiseño para la innovación ambiental de la tecnologia	ECOTECH-SUDOE	Luís Arroja
Aproveitamento energético da biomassa em recursos hídricos degradados ricos em microalgas	EnerBioAlgae	Margarida Coelho
poctep – cooperação transfronteirica Portugal-Espanha 2007-2013	acronym	local coordinator
Observatorio marino del margen ibérico v del litoral	RAIA.co	Jesus Dubert
Transferência de herramientas para la evaluación, ordenación, gestión y educación ambiental	TEAM-MIÑO	Isabel Lopes
en estuários		
Innovation Network Spain-Portugal – Rede de Transferência de conhecimento Universidade – Empresa.	INESPO	José Paulo Rainho
Rede Centro de Portugal - Castilha Y León		
life+ - project coordinated by UA	acronym	project coordinator
Conservatión of marine protected species in Mainland Portugal	MARPRO	Amadeu Soares
life+	acronym	local coordinator
Bussaco's recovery from invasions generating habitat threats	BRIGHT	Carlos Fonseca
lifelong learning	acronym	local coordinator
Competence assessment and development of potential entrepreneur	COMTRAIN	José Paulo Rainho
Turning European placements into a learning environment for entrepreneurial skills – as a key	UNIKEY	José Paulo Rainho
competence of graduates of European universities		
Improving hydrogen energy knowledge around European Union	KnowledgeH2	Fernando Marques
alfa	acronym	local coordinator
Información para la gestión de calidad de la docencia universitarla	ALFA III C.I.D.	Liliana Sousa
Gestión universitária integral del abandono	GUIA	Gillian Moreira



network of EU universities working with the UA in EU – funded projects started in 2011

intellectual property

intellectual property rights registration

	2009	2010	2011
copyright	4	10	6
logos	0	1	0
trademarks	14	20	20
design	1	0	0
national patents	21	17	16
international patents	28	23	3
utility models	0	1	0

intellectual property rights portfolio*



budget

research projects started in 2011

total budget by research centre and funding agency*

research centre	european union	foundation for science and technology	innovation agency	others	2010	2011
CBC		135.610			707.997	135.610
CESAM	2.667.410	3.661.400	542.584	273.135	7.077.397	7.144.529
CETAC MEDIA		184.037			403.133	184.037
CICECO	1.569.175	1.623.301			5.728.013	3.192.476
CIDMA		93.888			39,686	93.888
CIDTFF		225.219		5.000	638.636	230.219
CLC					180.000	
GEOBIOTEC		102.648	233.800		253,870	336,448
GOVCOPP			129.698		406.247	129.698
I3N	197.442	570.806			697.109	768.248
IEETA	918.747	52.038	849.236		1.456.949	1.820.021
INET-MD					105.000	
IT	944.661	1.434.355	262.639		5.380.716	2.641.654
Not integrated	665.888	126.312	216.191	644.097	1.129.970	1.652.487
QOPNA		284.260	367.125		778.868	651.385
TEMA	201.918	721.560			1.178.989	923,478
total	7.165.240	9.215.434	2.601.272	922.232	26.162.580	19.904.177





* Contracts with industry not included

approved budget under FCT projects

research centre	arts, humanities and social sciences	engineering	sciences	2010	2011
CBC			135.610	707.997	135.610
CESAM		97.020	3.564.380	4.624.631	3.661.400
CETAC MEDIA	184.037			115.125	184.037
CICECO		361.481	1.261.820	2.841.186	1.623.301
CIDMA			93.888	39.686	93.888
CIDTFF	225.219			389.412	225.219
CLC				130.000	
GEOBIOTEC			102.648	253.870	102.648
GOVCOPP				340.139	
I3N		48,882	521,924	669,509	570.806
IEETA		52.038		781.447	52.038
NET-MD				105.000	
Π		1.434.355		1.518.949	1.434.355
Not integrated	79.068	47.244		605.067	126.312
QOPNA	47.420		236.840	778.868	284.260
TEMA		721.560		1.178.989	721.560
total	535.744	2.762.580	5.917.110	15.079.875	9.215.434

approved budget under EU – funded projects

* Contracts with industry not included

european programmes	2010	2011
alfa		40.000
erasmus for young	14.000	
entrepreneurs		
espon	66.107	
FP7 – cooperation	3.882.560	2.401.476
FP7 — people	45.000	1.351.320
interreg – atlantic area	1.533.447	
interreg — sudoe		303.686
life+		1.674.116
lifelong learning		153,190
poctep		343.187
rfcs	540.562	898.265
sanco	112.900	
tempus	81.967	
total	6.276.543	7.165.240

people

staff by department

department	FTE	
university	2010	2011
department of environment and planning	18,6	18
department of biology	35,2	35,3
department of social sciences, policy and planning	26,5	27
department of communication and art	83	81,4
department of economics, management and industrial engineering	57,2	57,3
department of education	42,9	40
department of electronics, telecommunications and informatics	85,3	82,8
department of ceramics and glass engineering	17	17
department of civil engineering	19,9	19,4
department of mechanical engineering	30,8	28,9
department of physics	49,6	48,6
department of geosciences	14,5	14,5
department of languages and cultures	47,9	47,5
department of mathematics	67,5	66
department of chemistry	51,4	49,2
department of health sciences	14,7	17,2
sub-total	662	650,1
politechnical schools		
school of design, management and production technologies of aveiro north	14,5	14,9
school of health of the university of aveiro	42	43,9
águeda school of technology and management	54,4	48,8
school of accounting and administration of aveiro	75,5	71,6
sub-total	186,4	179,2
total	848,4	829,3

staff by category

	FTE	
category	2010	2011
university		
full professor	60,3	55,8
assotiate professor	119,3	118,3
assistant professor	365,4	371,9
lecturer	123.7	113,2
other teaching staff	17	17
researchers	106,4	102,4
post-doctoral students	125	83*
politechnical schools		
coordinator professor	12,1	11,6
adjunt professor	90,3	89,7
lecturer equivalent	60,3	51,8
total	1079,8	1014,7

*provisional data

Note: does not include free-of-charge or non-working teaching staff

PhD students by department

The statistic by department	PhD students *	
department	2010/2011	2011/2012**
department of environment and planning	63	74
department of biology	100	123
department of social sciences, policy and planning	19	22
department of communication and art	216	155
department of economics, management and industrial engineering	176	162
department of education	224	168
department of electronics, telecommunications and informatics	156	122
department of ceramics and glass engineering	44	64
department of civil engineering	26	35
department of mechanical engineering	40	63
department of physics	75	54
department of geosciences	22	18
department of languages and cultures	68	37
department of mathematics	37	30
department of chemistry	105	105
department of health sciences	47	36
total	1.330	1.142

* The students of joint doctoral studies are considered in each participating department, Therefore, the sum of the students by department is superior to the total, **provisional data

research centres

The University of Aveiro hosts 18 research centres, including 4 Associate Laboratories and 14 Research Units. Associate Laboratories are research units which demonstrate, in particular through the results of evaluation, the capacity to cooperate in a stable, competent and effective manner in carrying out specific objectives of the scientific and technological policy laid down by the Portuguese government.

These research centres are evaluated by the Portuguese Science and Technology Foundation (FCT) according to a system based on periodic assessment, by international experts, of reports and activity plans, including direct contacts with researchers and their institutions during visits to all units. This evaluation exercise culminates in the attribution of a qualitative grade which determines the volume of pluriannual funding to be received up to the next evaluation.

The most recent round of FCT evaluations took place in 2008, and the UA research centres were evaluated as follows.

evaluation of the UA's research centres



(1) good

- > UnIMeM Research Unit in Music and Musicology
- (2) fair
- CETAC.MEDIA Research Centre for Communication Technologies and Sciences
- CLC Centre for Languages and Cultures
- (8) excellent
- > CIDTFF Research Centre for Didactics and Technology in
- Teacher Education
- OPPA Organic Chemistry, Natural and Agro-food Products
- TEMA Centre for Mechanical Technology and Automation
- associate laboratories
- > CESAM Centre for Environmental and Marine Studies
- > CICECO Centre for Research in Ceramics and Composite Materials

I3N-FSCOSD Institute for Nanostructures, Nanomodelling and Nanofabricattion – Physics of Semiconductors, Optoelectronics and Disordered Systems

IT Instituto de Telecomunicações

(7) very good

CBC Centre for Cell Biology
 CIDMA Centre of Research and Development in Mathematics and Applications

GEOBIOTEC GeoBioSciences, GeoTechnologies and GeoEngineering
 GOVCOPP Governance, Competitiveness and Public Policies
 ID+ Research Institute for Design, Media and Culture

EETA Institute of Telematics and Electronic Engineering of Aveiro INET-MD The Ethnomusicology Institute – Centre for the Study of Music and Dance

RESEARCH SUPPORT OFFICE (GAI)



In order to reinforce European collaboration, UA strongly encourages its researchers to create ties with their colleagues in European countries, by responding jointly to calls for proposals for European programs. To achieve this goal, UA set up the **Research Support Office (GAI)**, with specialists and projects managers who can offer research centres at UA help in the development and implementation of strategies for research, in pursuit of the objectives established for the University and for the European Research Area, and individually assist UA researchers in the whole process. GAI provides researchers with:

> up-to-date information on national and international research programmes;

information on fellowship programs;

- > specific announcements of calls and events;
- > one-to-one coaching and support of proposal submission and project management;
- information events.

http://www.ua.pt/research http://www.facebook.com/pages/Research-Support-Office-GAIUA/300765536600188





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