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DE LA FACULTAD DE CIENCIA Y TECNOLOGÍA**

**VII JORNADAS DE PRESENTACIÓN
DE EMPRESAS Y CENTROS DE INNOVACIÓN TECNOLÓGICA**



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DEKANO ANDREAREN GUTUNA

Lankide agurgarriak,

Atsegintasunez iragartzen dizuet otsailaren 8, 9, eta 10ean ospatuko diren Zientzia eta Teknologia Fakultateko III. Ikerketa Jardunaldien eta VII. Enpresa Aurkezpen eta Teknologia Berrikuntza Zentroen Jardunaldien hurrengo edizioa.

Jardunaldi horien goiburua “Ikerketa, berrikuntza eta sinergia” da, eta hori dela eta, Fakultatearen pareko bideak garatzen dituzten ikerketa zentroak gonbidatu ditugu Jardunaldietan parte har dezaten, helburua gure Fakultatean ikerketa eta berrikuntza sustatzen dituzten sinergiak sortzea delarik.

Alde batetik, Jardunaldien helburua ikasleriari Fakultateko Talde ezberdinek burutzen duten ikerketa erakustea da, beren ikertzaile bokazioa pizteko asmoz. Beste alde batetik, hainbat kasutan egin den antzera, zenbait enpresek eta teknologia berrikuntza zentroek ikasleek lan munduan sartzeko dituzten aukerak eta baldintzak aurkeztuko dizkiete azken mailako ikasleei. Jardunaldi horiekin lotu nahi diren helburuen garrantzia kontuan hartuta, zuen parte hartze aktiboa eskatzen dizuegu, eta baita zuen ikasleena ere, klaseko bertaratzea Jardunaldietara aldatuz.

Azkenik, hurrengo parte hartzeekin kontaktzen dugula adierazi nahi dugu: inaugurazio-hitzaldia eskainiko duen Fernando P. Cossio Doktorea, Ikerbasque Fundazioaren Lehendakaria; eta Jardunaldien inaugurazio-ekitaldiaren buru izango diren Eusko Jaurlaritzako Zientzia Politikarako Zuzendaria, Begoña Ochoa, eta Berrikuntza Errektoreordea, Miguel Ángel Gutiérrez.

Parte hartzera animatzen zaituztet, aurreko edizioetan bezala, ekimen hau arrakasta handikoa izan dadin.

Agur bero bat,

Esther Domínguez
Zientzia eta Teknologia Fakultateko Dekano Andrea

CARTA DE LA DECANA

Estimadas compañeras, estimados compañeros,

Me es grato anunciaros la próxima edición de las III Jornadas de Investigación y VII Jornadas de Presentación de Empresas y Centros de Innovación Tecnológica de la Facultad de Ciencia y Tecnología, que tendrán lugar los días 8, 9 y 10 de febrero.

El lema de estas Jornadas es “Investigación, innovación, sinergias” y en ese sentido, hemos invitado a participar a centros de investigación que desarrollan líneas afines a la Facultad, con el objetivo de crear sinergias que impulsen la investigación y la innovación en nuestra Facultad.

El objetivo de estas Jornadas es por una parte mostrar a nuestro alumnado la investigación que llevan a cabo los diferentes Grupos de la Facultad, de cara a despertar vocaciones investigadoras. Por otro lado, como en otras ocasiones, varias empresas y centros de innovación tecnológica presentarán al alumnado de los últimos cursos las posibilidades y los requisitos para su incorporación al mundo laboral. Dada la importancia de los objetivos que se pretenden con estas Jornadas, os pedimos que participéis activamente en las mismas y promováis la participación de vuestro alumnado, trasladando la presencialidad del aula a las Jornadas.

Finalmente, indicar que contamos con la participación del Dr. Fernando P. Cossio, Presidente de la Fundación Ikerbasque que impartirá la conferencia inaugural, así como de la Directora de Política Científica del Gobierno Vasco, Begoña Ochoa y del Vicerrector de Investigación, Miguel Ángel Gutiérrez, que presidirán el Acto de Inauguración de las Jornadas.

Os animo a todos a participar para que esta iniciativa sea un éxito como lo fue en ediciones anteriores.

Recibid un cordial saludo,


Esther Domínguez
Decana de la Facultad de Ciencia y Tecnología

ZIENTZIA ETA TEKNOLOGIA FAKULTATEKO III. IKERKETA JARDUNALDIAK
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2012 OTSAILAK 8-9-10 de FEBRERO

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RESÚMENES/ABSTRACTS



Bio Zientziak/Biociencias

ENAF-Efficiency of nitrogen use and effect of mycorrhization in agroforestry systems

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KEY WORDS: abiotic stress, ammonium nutrition, biotic stress, bread making quality, CH₄, fertilization, grain proteins, greenhouse gases emission, mycorrhiza, nitrification inhibitors, N₂O, nitrogen metabolism

The group "ENAF- Efficiency of nitrogen and effect of mycorrhization in agroforestry systems: yield, quality and environmental impact minimization" has as general objective to deepen into basic scientific knowledge (metabolic, physiological and molecular aspects within the soil-plant system), while looking for practical applications, which will help in decision making on the rational use of fertilizers and phytosanitary products, with the long term aim of contributing to a production system focused on quality while minimizing environmental impact.

1. Nitrogen use efficiency by crops: agronomic, environmental and physiological aspects.

Nitrogen fertilizer application is needed in order to achieve good crop yields. Nevertheless, the excessive use of nitrogen fertilizers leads to environmental problems such as water pollution by nitrate leaching and global warming by greenhouse gases emissions. If a sustainable production system is to be achieved, it is necessary, on one hand, to understand the processes related to N transformations in the soil and the physiological and molecular mechanisms that can lead to an increase in nitrogen use efficiency by plants, and, on the other hand, to translate this knowledge into a good agronomic management system, which includes the development of ammonium-based fertilizers together with nitrification inhibitors or the splitting of fertilizer application according to the crop needs. The ENAF group deals with this matter both from an environmental point of view as well as from the knowledge of plants' biochemistry and physiology, in order to achieve a better crop quality.

2. Improving the quality of Reproduction Forestry Materials to be used in re-forestation

Within the forestry line, the ENAF group has developed an optimized technique of vegetative propagation of the most economically interesting forestry species in the Basque Country, *Pinus radiata* D. Don. These techniques will allow the production at the nursery of plants previously selected in terms of their quality regarding several factors (response to biotic and abiotic stresses, wood quality, etc.). The group puts emphasis in the inoculation of the plant material with ectomycorrhizal fungi due to the beneficial role of these organisms on the modulation of the response of the plants to environmentally adverse conditions. In this sense, most of our efforts have been focused into the study of the effect of mycorrhization on the tolerance of *P. radiata* to drought and on water use efficiency, and we have begun a study at both the histological and molecular levels regarding the response of *P. radiata* to the biotic stress caused by the fungus *Fusarium circinatum*. A better understanding of the nature and mechanisms involved in the plant-pathogen interaction could be very useful in the control of this disease.

Colaborations: Universidad Pública de Navarra (UPNa), Escuelas Técnicas Superiores de Ingenieros Agrónomos de la Universidad Politécnica de Madrid y de la Universidad de Córdoba, SERIDA (Organismo Público de Investigación del Gobierno del Principado de Asturias), NEIKER-Tecnalia, Intia S.A., BASALAN (Diputación Foral de Bizkaia), Estación Experimental del Zaidín-CSIC, Universidade de Lisboa, red RUENA (Red para el uso eficiente del nitrógeno en la agricultura), Grupo Roullier, K+S Wachstum Erleben, INRA-Versailles, BC³ Basque Center for Climate Change.

Aknowledgements: Grupo de investigación Consolidado UPV/EHU y Gobierno Vasco (IT526-10), MCINN AGL2009-13339-CO2-01/AGR, MICINN-INIA RTA2009-00028-CO3-03, K-Egokitzen II-Cambio climático (IE10-277), Gobierno Vasco-UPV/EHU PA09/07, PA11/03 y PA11/04, K plus S Iberia S.L. y UPV/EHU 2011.0051.

Ecophysiology of plant stress and soil contamination (EKOFISKO)

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KEY WORDS: Environmental Stress, Biomarkers, Extreme environments, Nutraceutic, Photoprotection, Phytoremediation, Soil contamination, Revegetation, Global Change.

Since 1990 The EKOFISKO group has developed research and teaching activities on physiological and ecophysiological aspects of natural and anthropic agents causing stress in plants. Our group is a consolidated research group distinguished with the highest grade of the Basque Government classification for Scientific Groups. The group is composed of 7 PhD, 3 PhD students and 3 degree students.

This group has developed a variety of novel methodological tools: (i) determination of plant stress biomarkers, in particular those related to photoprotection and oxidative stress, (ii) set up of plant toxicity bioassays to determine the ecotoxicological effects of pollutants in contaminated soils, and (iii) implementation of physiological parameters to evaluate phytotoxicity or damage caused by natural stress conditions as extreme temperatures, drought, light intensity, nutritional disorders, etc. Recently, in collaboration with other groups, we have incorporated genomic methodologies with emphasis in differential gene expression and in the application of DNA microarrays to assess and monitor soil health in a multidisciplinary approach.

All these methodologies have been implemented in several more applied research areas:

- Determination of the role of photoprotective compounds and tolerance to stress conditions (natural or anthropic) with particular emphasis on the acclimation to extreme environmental conditions, such as those prevailing at high altitudes, forest understory or historically polluted sites.
- Use of plant biomarkers to monitor environmental and global change and genotype plant selection for tolerance to adverse climatic agents and phytoremediation.
- Identification of environmental agents to enhance nutraceutical compounds (carotenoids and tocopherols) in plant foods.
- Use of plants for ecological restoration of degraded environments, specially polluted soils through ecotechnologies as bio- and phytoremediation (phytostabilization, phytoextraction and rhizodegradation).
- Assessment and monitoring soil health with biological indicators, during remediation processes.

The research indicated above is currently carried out in a multidisciplinary approach in collaboration with relevant national and international scientists, universities (Complutense de Madrid, Autónoma de Barcelona, La Laguna, Helsinki, La Frontera, Tartu, Australian National) and institutions (Neiker, Gaiker, Phytosphere Institute, Royal Kew Gardens, USDA, etc), and supported regularly by many competitive projects. The quality of group's achievements is supported by regular publications in international journals (42 in the last 5 years), and by regular participation in national and international congresses. We also have a compromise on the cooperation for development, with several projects in Latin American universities (Chile, Nicaragua and Cuba). Besides, not only our group is very active in the formation of PhD students (5 PhD in the last 5 years), but also we participate in three Official Master Programs: "Agrobiología Ambiental", Environmental Contamination and Toxicology and "Enología Innovadora" and in the Doctorate Program "Agrobiología Ambiental" honoured with a quality award by the Ministry of Education.

Plant adaptations to climate change and their use as CO₂ sinks and bioenergetic crops.

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KEY WORDS: Bioenergetic crops, climate change, CO₂ sinks, plant physiology and production.

Climate change raises important scientific challenges for plant physiologists. Firstly, we need to expand and broaden our knowledge about the responses of plants to the environment, so that we can predict the impact of climate change on the growth of the crops and natural ecosystems. Secondly, the understanding of the response of the plants to climate change provides us tools and knowledge to minimize the negative impact.

The rise of CO₂ may alter the global climate raising temperature and modifying the rainfall pattern exacerbating even more the risk of drought and salinity, especially in the Mediterranean region, reducing drastically the productivity of the crops. Furthermore, these alterations can also modify the interactions between plants, provoking variations in biodiversity.

In consequence, one of the main uncertainties when analysing the global impact of climate change in the productivity of agroforestry and of ecosystem is the response of the plants to elevated CO₂ in combination with other environmental stresses and changes of species dominance in the ecosystems.

Plants through photosynthetic activity function as excellent sinks of environmental CO₂ reducing the effects of climate change and contributing to the Kyoto compliance. On the other hand, the produced biomass could have an energetic use. However, those perspectives can be altered by factors such as limitation of nutrients and water, temperature rise, salt stress and/or other factors related to the rise of CO₂ that can affect physiology and productivity of the plants.

Thus, the objective of this research group is focused on the analysis of different factors that affect physiology, growth and productivity of the plants in the nowadays changing environment such as atmospheric CO₂, water availability, soil salinization, NO₃⁻ availability, as well as interactions within them and plant-plant interactions. We also investigate if the plants will be able to adapt to these new environmental conditions.

At the same time, we intend to take advantage of the capacity of the plants themselves to kidnap the excess of environmental CO₂ permitting that way a longer period of C retaining, eventually using plants as biomass source for utilization as renewable bio-fuels.

Presence of selected toxic microalgae species in the Southeastern Bay of Biscay

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KEY WORDS: microalgae, phytoplankton, taxonomy, toxicity.

Many small fast running rivers drain to the Bay of Biscay in the Northern coast of Spain where river plumes constitute a preferable area for the Bay of Biscay anchovy, one of the main marine resources of the region. In the eastern side of this coast, phytoplankton has been regularly monitored in 25 estuaries and the adjacent coastal waters. These monitoring data have revealed that the toxic diatom *Pseudo-nitzschia* spp. is a dominant component of the phytoplankton in the outer part of the estuaries and on the coast, reaching frequently values about 10^5 cells L^{-1} in spring and summer. The aim of this research is to gain insight into the diversity of the genus *Pseudo-nitzschia* in coastal waters of the Southern Bay of Biscay where there is a lack of data on the taxonomic composition of these potentially toxic diatoms. The study focuses on the Nervion River estuary, which is one of the largest estuaries of the region. In the last decade, the estuary has experienced a marked increase in water quality after the implementation of a wastewater treatment program.

On the other hand, potentially toxic benthic microalgae have been the subject of much research work in the last years and the methodology used to identify them, firstly molecular methods and electron microscopy, have allowed to gain insight into their taxonomy from a broad range of marine areas. These benthic algae, although epiphytic on macroalgae, can swim forming blooms in the water column of the beaches, thus constituting a risk for bathers.

Both kinds of potentially toxic microalgae are being studied by means of ultrastructural analyses and molecular methods in order to know the morphological as well as genetic diversity.

Study of structural and functional diversity for a sustainable land management

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KEY WORDS: Biodiversity, Ecosystem services, Mapping, Models, Surveys

Human well-being and progress towards sustainable development depends mainly on the improvement of ecosystem management, since as demands for services supplied by the ecosystems grows human activities diminish the ability of many of them to meet such demands.

The aim of our research is to analyze the structure and functioning of the socio-ecosystems in order to provide the information required by the decision-makers for a sustainable land management, i.e. maintenance and improvement of ecosystems and their biodiversity.

The methodologies used are the following:

- Analyze the state and evolution of ecosystems and their provision of services in the last decades by means of different types of indicators.
- Quantify and value Biodiversity and some ecosystem functions and services at different spatial scales (CAPV, Bizkaia, Lea watershed , Urdaibai...), using GIS programs, for the sustainable land management. Some of these services are: Carbon storage, Water Flow Regulation, Erosion control or Recreational use.
- Study the perception of the local communities that are the main beneficiaries of the services provided by ecosystems, by means of surveys.
- Analyze future stakeholders-defined scenarios of the territory through the use of models (CO₂Fix, ARIES...), mainly for improving a sustainable land management.

Diversity, Ecology and Conservation of Macrofungi

Isabel Salcedo Larralde, Esti Sarrionandia Areitio, Nerea Abrego Antia, Asier Uribeetxebarria Alonso de Armíño
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KEY WORDS: Basque Country, Mycology, Macrofungi, Mycorrhizas.

Fungi are an important and diverse group of organisms, which play vital roles in ecosystems. Fungi are essential to such processes as decomposition, nutrient cycle and nutrient transport. In this way, fungi encompass a heterogeneous group of organisms with different life strategies and very diverse interactions. Taking into account the estimation of Hawksworth (1991) only 5% of the fungal species of the World has been described, and furthermore little is known about their ecology.

With the aim of knowing the diversity of fungi, one line of research in the group of Mycology has centred on the knowledge of the diversity of macromycetes, especially Basidiomycota. During the last years, in collaboration with research of the Botanical Gardens of Madrid and Lisbon, the study has been focused on corticioid fungi, as well as on the study of the order Cantharellales (PhD *The order Cantharellales in the Iberian Peninsula and the Balearic Islands* carried out by Ibai Olariaga). However, during the last six years we have started to study the corticioid fungi of the Macaronesian region, where besides cataloguing the mycobiota of the territory, we try to analyze their biogeographic interconnections (Part I. Azores, Madeira and Canary Islands. Part II. Cape Verde and the northwest coast of Africa).

From an ecological point of view we have carried out mycoceonological studies that allow us to know the diversity of particular ecosystems, which are the basis of management programmes. In the same way, we have begun the study of lignicolous fungal communities, with the PhD titled *Lignicolous macromycetes in beechwood of Navarre: diversity, ecology and conservation* (Nerea Abrego). Among the main objectives of this study are to know the diversity of the lignicolous macromycetes of beechwoods, as well as to determine the main factors that affect this diversity, and subsequently set out some guidelines for a more sustainable forest management.

Another important role of fungi are mycorrhizal associations, which compose complex relationships in land ecosystems at root level. In this way, *Alnus* is one of the few genera which is able to establish three types of mutualist associations in their roots (2 of them are mycorrhizas), and this is why its species are pioneers, fast-growing, and able to grow in extreme conditions. Alder forests are essential for river ecosystems, and taking into consideration the little data available about the mycorrhizal fungi associated with alder, we have considered analyzing this diversity in the Basque Country.

Finally, we want to mention the project *Evaluation of the threat level of the threatened species from the preliminary Red List of Fungi of the Basque Country* financed by Ihohe and carried out by our group.

Genomic and proteomic approaches to Cancer Biology

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KEY WORDS: Cancer, Cell Cycle, Cell Signaling, Gene knockout, E2F, Gene Expression, Genomics, Proteomics.

Cells receive signals for proliferation through growth factor receptors located at their plasma membrane. The signal is transduced inside the cell by signaling molecules that change the cellular state, leading to responses at the nuclear level. Cellular proliferation requires duplication of the nuclear content and physical division of the cell. This process of cell growth and division, called the cell cycle, is the fundamental means by which all living organisms propagate. It must be exquisitely controlled, because aberrant cellular proliferation may give rise to pathologies such as cancer or autoimmunity.

Our understanding of cell cycle control increased enormously with the identification of a system that coordinates the cell cycle to make it work as a clock, and that is conserved in all eukaryotes. However, two major questions remain unsolved: How does this machinery integrate and process growth-controlling signals and decide on the cell's fate? And how is this decision executed?

Research in Biomedicine has experienced an extraordinary revolution in recent years, with the development of technologies that allow the analysis of complete sets of genes and proteins in a particular cell or organism. This has led to the birth of the novel fields of Genomics and Proteomics.

We are applying genomic and proteomic approaches, together with classical methods of genetic analysis, to identify the proteins and pathways that play a key role in the control of cellular proliferation and cell fate, including the dysregulation that contributes to oncogenesis. Current areas of research in the laboratory include:

- 1. The signaling pathways that mediate cellular proliferation, with an emphasis on Ras/Rac-dependent signal transduction.**
- 2. The components of the cell cycle that integrate and process growth-regulatory signals. This area focuses mainly on the analysis of E2F transcription factor activities.**

Understanding the role of small GTPases of the Rho family in P2X₇ receptor-mediated signaling in macrophages

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KEY WORDS: Small GTPases, P2X₇ purinergic receptor, ATP, intracellular signaling. Macrophages

SUMMARY OF THE RESEARCH PROJECT

The small GTPases of the Rho family are involved in many cellular processes, such as the control of cytoskeleton events, vesicle trafficking, cell cycle control and among other, cell apoptosis. The best characterized members in a biochemical point of view are RhoA, Rac1 and Cdc42. In the last few years we have deciphered different relevant events related with the P2X₇-receptor in cellular models and macrophages, including the Reactive Oxygen Species (ROS) generation and Mitochondrial Membrane Depolarization (MMD) which can contribute together with massive influx of Ca²⁺ to cell death. These observations have led us to hypothesize that the generation of ROS and MMD induced by P2X₇ receptor in macrophages could be carried out by the involvement of these monomeric G proteins. Therefore, we have decided to raise the next objectives:

1- **To study the kinetics of activation of the small GTPases of the Rho family, specificity, regulation and effector molecules involved in transducing signals emanated from the activated P2X₇-receptor**, in rat SMG cells, murine RAW 267.4 cell line, and peritoneal macrophages from C57BL mouse. We will characterize the P2X₇ receptor pharmacology on small GTPases of the Rho family (Rho A, Rac1, Rac2 and Cdc42) activation using receptor agonists such as ATP and Bz-ATP and inhibitors. We also will determine the involvement of other purinergic receptor and the contribution of P2X₇R will be determined in isolated SMG cells in suspension and culture. According with our previous studies P2X₇R is the main purinergic receptor in SMG cells, however in macrophages we will determine the importance of P2X₇ contribution on small GTPases signaling pathways and ROS production over other purinergic receptors expressed by the cell.

2- **To understand the function of the Rho family GTPases on ROS generation in response to the P2X₇-receptor activation, dependency on calcium and/or sodium requirement.** The subpool of P2X₇ receptor involved in Rho GTPases/ROS production pathway and calcium dependence will be determined by using specific inhibitors of N-sphingomyelinase such GSH and GW4869, this enzyme is coupled to P2X₇ receptor in raft microdomains. Coupling studies on P2X₇ and Rho GTPases activation and subsequent ROS production, together with transient transfection of ODNs (oligodeoxynucleotides) will be determined in SMG cells and macrophages.

3- **Implication of P2X₇-receptor/Rho GTPases/ROS generation in the apoptosis program in macrophages.** Apoptosis indicators such as release of cit c, caspases activation, DNA fragmentation and cell doubled staining with Annexin V-FITC and propidium iodide and analysed on a FACScan will be determined in cells exposed to ATP and analogues.

METHODS:

FLUORESCENCE ANALYSIS: cells will be excited alternatively every 350ms (1s interval) at 340 and 380 nm on the stage of a Nikon TE300 microscope equipped with a DeltaRAM system Image Master from PTI by using a live-cell imaging system coupled to a perfusion chamber at 37°C. Other assays will be performed in a conventional fluorimeter Aminco Bowman-2. ELISA, Immunoprecipitation, SDS-PAGE, Western Blot, Plasmids constructions, DNA transfections, Affinity precipitation of proteins bound to active GTPases, Apoptosis assay.

Development and application of proteomic technology

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KEY WORDS: proteomics, E2F2, phosphorylation

Proteomics refers to large-scale analysis of proteins, including protein identification, expression analysis, post-translational modifications and protein-protein interactions, with the aim of elucidating a general and integral view of protein networks and cellular and pathological processes. Our group is involved in proteomics studies in two aspects. On one hand, we develop methodology in order to provide the Proteomics Facility with new services to offer. On the other, we use established proteomics approaches to tackle biological issues such as the ones related to the transcription factor E2F2.

- Protein identification is the basis of proteomics. A search engine uses data obtained by mass spectrometry (MS) to identify proteins from a sequence database. A strategy based on tandem MS allows the identification of proteins from mixtures. At the beginning, and somehow restricted by the technology we had in hand, we were able to identify proteins from purified samples and to analyse components of protein complexes and protein-protein interactions. As the result of the acquisition of new instrumentation we have extended our capabilities and can analyse complex protein mixtures, such as cell compartments and total cell extracts from which we are able to identify a few hundred proteins. Nevertheless, more in deep analysis, identifying a few thousands of proteins, has been shown to be feasible and we are trying to reinforce our methodology in order to reach those values.
- Very often, the protein contents of a number of samples need to be compared, for instance disease/normal or treated/non-treated. In order to do that, proteins need to be quantified as well as identified. The pioneer technique for this purpose has been based in two-dimensional electrophoresis (2DE) and although it is still a powerful everyday methodology new MS-based approaches are being developed and are nowadays confirmed as reliable methods for either relative or absolute quantification. Among these new methodologies label-free quantification is certainly standing out. We are applying this technology in our laboratory and the quantitative results are being very satisfactory. On the other hand, development of methods for targeted quantitative proteomics is one of the challenges we have in the near future.
- Phosphorylation has an important role in protein function. MS analysis of protein phosphorylation is not trivial due to low stoichiometry and ionisation efficiency issues. Therefore, phosphopeptides need to be enriched prior to MS analysis. Our group works on phosphopeptide enrichment methods based on titanium dioxide.
- We are applying all the technological developments mentioned above to the analysis of the E2F transcription factors. This work is being carried out in collaboration with Ana Zubiaga's Group (Genetics Department). E2F2 interacts with other proteins to carry out its function. Identifying those interacting partners may help us have a better understanding of the role of this transcription factor. Thus, immunoprecipitation with E2F2 specific antibodies or oligoprecipitation using sequences recognised by E2F2 is performed and the outcome is analysed by LC-MS/MS. This kind of analysis has led to the identification of ALY as a protein that modulates the transcription of E2F target genes involved in cell cycle.

Genomics and Health: Disentangling complex diseases in humans and animals

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KEY WORDS: genomics, candidate genes, gene expression, infectious diseases, obesity, eating disorders, disease resistance.

*** Genetic basis of infectious diseases in animals**

We are involved in the analysis of the genetic basis of infectious diseases with viral aetiology in domestic and non-model animals. In this area we have two main scientific goals: The search for functional polymorphisms affecting the immune response and the study of the influence of host genetics in the pathogenesis of infectious diseases and cancer. Currently we seek to contribute to the clarification of some aspects of the pathogenesis of two viral diseases, Ovine Pulmonary Adenocarcinoma and Maedi-Visna. We have analyzed a number of candidate genes of both the innate and adaptive immunity with different markers and techniques (Sequence Based Typing, Microsatellites, SNPs) and their expression in different tissues. Association between markers and disease development has been tested employing logistic regression, taking into account marker type, sample size and structuration and statistically significant results have been detected for some of them (cytokines, TLRs and other additional innate immunity genes). In a next step, we will aim to fully characterize those genes in order to identify the causal polymorphisms and the mechanisms with which they confer Resistance/Susceptibility to disease progression.

On the other hand, we are also interested in the analysis of endogenous retroviruses (ERVs), genomic elements with retroviral origin which can have both beneficial (resistance to infectious counterparts) and adverse effects (may cause disease) in the host. Given the amount of genomic information currently available following the complete sequencing of various genomes, we have carried out a multi-species genomic analysis to identify retroviral elements inserted in these genomes. We have characterized their evolutionary dynamics and their possible expression and functional role by means of bioinformatic methods. Now, we have started to detect and characterize retroviral elements specifically in the sheep genome by molecular techniques such as PCR suppression and iPCR. We will also analyze their expression in different tissues in healthy and diseased animals.

We hope that our research will open new channels for the elimination of infectious diseases affecting livestock.

*** Eating behaviour, phenotype and genetics in humans**

Obesity and its associated comorbidities, such as diabetes, cancer and coronary heart disease, represent one of the biggest public health challenges today. The marked rise in obesity observed over the last years suggested that behavioral and environmental factors underpin the mismatch between energy intake and energy expenditure. However, not all individuals become obese, suggesting that there is considerable variation in responsiveness to "obesogenic" environments. The epidemiology of obesity suggests that, for the majority of individuals, the disorder arises from an interaction between genetic predisposition and lifestyle behaviors such as dietary intake and physical activity. The heritability of body weight is high, and genetic variation plays a major role in determining the interindividual differences in susceptibility or resistance to the obesogenic environment.

We are now detecting obesogenic environmental factors in working populations, including a gender perspective. Moreover, we are also characterizing obese phenotypes based on BMI and other parameters in a specific working population. In order to investigate how genetic and behavioral risk factors combine to lead to excess weight gain, our next goal will be the detection of associations between the genetic variation in some candidate genes and the obese and pre-obese phenotypes, as well as the interactions with the environmental factors.

Genomic Resources

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KEY WORDS: Genetic markers, Population genetics, Genetic association studies, NGS

"Genomic resources" is a Consolidated Research Group for the Department of Education, Universities and Research of the Basque Government (2010-2015). The group has 3 main lines of research where the genome analysis applies to 1) improve the management of the marine environment, especially of fisheries and mariculture species, 2) improve the management of farms, semi-wild species and hunting land species, 3) identification of genes associated with traits of interest, such as susceptibility / resistance to bacterial infections. To carry out the research objectives we have expertise in two disciplines:

1. POPULATION GENETICS/GENOMICS

In this research area we are focused on the genetic characterization of local animal populations and individual "DNA fingerprinting" through DNA markers and sequences. In the first case, we try to establish species' taxonomy and evolution, the population genetic structure, intra- and inter-population diversity, hybridization and introgression processes as to provide useful information for species management and conservation strategies. The "DNA fingerprint", the exclusive genetic information of an individual, allows carrying out parentage testing in animals and humans, the assignation of an individual to a certain species/breed/population, the identification of Genetic Modified Organisms (GMO), and the traceability of individuals and their products, all of them applications in areas such as Animal Conservation and Genetic Improvement, Animal Resources Management, Plague Treatment, Food Safety and Forensic Genetics.

2. GENETIC ASSOCIATION STUDIES

The general objective of this research area is the identification, by candidate gene or whole genome approaches, of genetic markers involved in the phenotypic variability of several human and animal traits such as: susceptibility/resistance to autoimmune human diseases (Antiphospholipid Syndrome), and economically important animal traits (resistance to bovine paratuberculosis and mariculture species growth). These associated genetic markers are useful tools for an individualized human medicine, since diagnostic, prognostic and/or therapeutic markers can be identified. In animals, the identified markers can be used in Marker Assisted Selection (MAS) or Genomic Selection based breeding programs, with the aim of obtaining individuals with a higher economic value.

In this sense, we have succeeded in applying genetic markers to address specific questions in those disciplines for human, domestic and wildlife animals and plant species, such as: *Ovis aries* (sheep), *Bos taurus* (cattle), *Equus caballus* (horse), *Apis mellifera* (bee), *Reticulitermes spp.* (termite), *Lepus spp.* (hare), *Cervus elaphus* (deer), *Canis familiaris* (dog), *Engraulis encrasicolus* (anchovy), *Thunnus spp.* (tuna fish) and *Zea mays* (corn),.... Furthermore, as the majority of species we are dealing with currently, such as anchovy or tuna species, are non-model organism (lack a reference genome) the group is specializing in the application of massive parallel sequencing (also called Next Generation Sequencing or NGS, techniques such as Roche's 454 technology and Illumina's HiSeq one) for the reduced representation sequencing of the genome, the discovery of SNP markers, differential gene expression studies and genome annotation in these species in order to optimize management and allow genetic improvement in breeding programs.

Gene Flow Processes in South America.

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KEY WORDS: Gene Flow, Alu insertions, South America

In the last years, we have approached the genetic characterization of several South American populations in different studies, to assess the impact of varying levels of gene flow on the genetic background of the human groups examined.

We have selected for this purpose the polymorphic Alu insertions. Alu elements are very useful molecular markers for the reconstruction of both past human demographic events and evolutionary history, since they are stable polymorphisms with a known ancestral state. Furthermore, they are neutral from the selective viewpoint and have identity by descent not just by state.

The populations analyzed so far are:

Mestizos from Antioquia (Colombia), resulting from matings between Native American people, European settlers and African slaves. This population has experienced intense gene flow processes, hence showing a high degree of genetic admixture.

Afro-descendants from Antioquia (Colombia), whose ancestors arrived on the American continent as slaves. The gene pool of Afro-descendants shows a low level of Amerindian component and no traces of admixture with people of European ancestry. Thus, genetic data indicate that the intensity of the gene flow has traditionally been lower in Afro-descendants than in Mestizos, presumably due to the origin of many of their communities, composed of runaway slaves characterized by a marked reluctance to cultural and genetic contacts with other human groups.

Amerindians of Jujuy (Argentina), particularly those living at the highest altitudes of the region, and therefore, with a difficult access. This situation has resulted in a considerable isolation of the population. Gene flow has differentially affected the different geographical regions of Jujuy, resulting in a declining trend of genetic admixture according to altitude: from substantial admixture rates in the lowlands to almost no admixture in the highest region (La Puna).

The Waorani (Ecuadorian Amazon) constitute an ethnic group with a historically reduced population size and highly isolated, mainly because of sociocultural reasons: an important component of population mortality is associated with internal quarrels, violence and warfare episodes between neighboring groups within the tribe, and the singularity of their language. Consequently, we have detected a significant loss of genetic diversity, probably due to recurrent bottleneck processes and high inbreeding levels.

Human Genetic Evolution

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KEY WORDS: ancient DNA, degraded DNA, mitochondrial DNA, forensic analysis, bioanthropology, melanoma, genetic expression, human diversity, resequencing, bioinformatics.

aDNA: RECONSTRUCTION OF THE EVOLUTIONARY HISTORY OF EUROPE

The general goal of this research is the reconstruction of the European evolutionary history through the genomic analysis of several Paleolithic and Neolithic sites located in the East of Europe. The paleogenomic data from these eastern Europe populations will allow us to contrast models and inferences previously done based both on prehistoric populations from Western Europe and in present day European populations.

Referring to the Neolithic period, the mtDNA studies from ancient human remains from European prehistoric sites reflect the complexity of this process, rejecting the extreme models of diffusion of Neolithic into Europe. Moreover, the reconstruction of the evolutionary history of Europe is undertaken including a region of Europe closely related to the main migratory process of *Homo sapiens*, with the analysis of the more ancient human remains from the early Paleolithic.

PIGMENTATION OF THE SKIN AND MELANOMA

There are genetic and environmental factors that determine the risk to melanoma susceptibility. In particular, light-skinned individuals are less protected against photocarcinogenesis and/or photoaging after solar irradiation, especially in recent years, when UV radiation has increased due to the weakening of the ozone layer. Therefore, we are trying to identify genetic variation associated with skin pigmentation in humans, in order to infer its adaptive value and assess its biomedical implications. For that reason, we are focusing on the detection of differentially expressed genes in melanocytic cell lines from individuals with different skin pigmentation, using expression chips (Affymetrix). Subsequently, a subset of loci is selected to analyze their sequence diversity by resequencing and their variation in the copy number of their exons. The variability discovered is analyzed in collaboration with other laboratories, in melanoma patients and healthy individuals. We are evaluating the adaptive value of these polymorphisms by means of bioinformatics and trying to infer the potential biomedical implications (predisposition to cutaneous melanoma).

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Bioanthropology of obesity, in gypsy population and in general population.

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KEY WORDS: obesity, Roma people, environmental factors, genetic factors, phenotype, case-control.

INTRODUCTION

Common obesity is an unfavorable condition characterized by a high body weight due to an excess of adipose tissue. Obesity is also one of the most important public health problems since it has been associated with the development of a number of metabolic alterations such as impaired glucose tolerance, type II diabetes, hypertension and cardiovascular diseases or sleep apnea.

In the last decades, obesity and overweight have reached epidemic proportions in many developed countries due to increased food availability and a more sedentary lifestyle. Obesity is a complex health problem and a social illness indicator. The causes of obesity have both genetic and environmental components, in fact, obesity is a complex multifactorial disease caused by the interactions of genetic and environmental factors. Although, genetic factors affecting obesity play an important role in the mechanisms leading to these metabolic disorder, obesity related inequalities among different populations might decrease through individual and social lifestyle changes.

OBJETIVES

The main objectives of this research are: (1) Determine the relative influence of genetic and environmental factors, in different obesity phenotypes. (2) Analyze the level of development and different types of obesity according to the environmental factors in different population groups. (3) Identify susceptibility genes for obesity: association analysis of the different alleles of candidate genes with different phenotypes of obesity.

METHODS

The sample was collected using two types of sampling design. Among Roma population, extended pedigrees were sampled, including some very complex 4 generation pedigrees. On the other hand, among general population, both obese and no obese individuals have been collected to conduct a case-control study.

In both cases, the acquired data included three different types of information:

- **Environmental assessment.** Background, lifestyle and socioeconomic data were collected through a personal survey.
- **Phenotype assessment.** The phenotype of each person was obtained by using different anthropometric measures.
- **Genetic assessment.** A sample of blood or saliva was collected to obtain the genotype of each person.

Both univariate and bivariate methods were used to assess quantitative genetics. For the genetic association analysis a number of candidate gene SNPs were selected from the NCBI data and HapMap. The DNA was extracted from saliva or blood samples and genotyped by TaqMan technology.

The programs used in this research were: Sequential Oligogenic Linkage Analysis Routines (SOLAR), SNPbrowser, SPSS v18.0, Microsoft Excel 2010 and TaqMan Genotyper Software.

The basis for inter-individual differences of growth in bivalves: a combined physiological and genetic approach.

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KEY WORDS: Bivalve, Growth rate, inter-individual differences, genotypic differences, candidate genes.

The growth performance of seeds (juvenile individuals) is one of the most important issues of bivalve aquaculture. Growth rate is the result of a balance between processes of energy gain and losses which is regulated by both endogenous (genetic) and exogenous (environmental) factors. Significant improvements in molluscs aquaculture might be obtained by, a) understanding the physiological characteristics that lead to a faster growth and, b) identification of the genes involved in such characteristics. These two research lines are currently being developed in our laboratory.

A) Experiments of physiological energetics have been performed with fast (F) and slow (S) growing seeds belonging to different bivalve species (*Ruditapes philippinarum*, *Crassostrea gigas* and *Mytilus galloprovincialis*). Results of all experiments indicate that fast grower seeds take advantage by means of:

- Higher clearance rates (filtering activity) derived from higher gill areas.
- Similar absorption efficiencies despite of ingesting a higher amount of food, this is, a higher digestive performance.
- Higher metabolic efficiencies that enable lower metabolic expenditures per unit of absorbed food.

B) To understand the genetic basis underlying the observed inter-individual physiological traits in seeds of the clam *Ruditapes philippinarum*, a RNA-seq experiment was designed. Using 1GB of data obtained from 454-FLX+ platform, a reference transcriptome is currently been created combining mRNA from different life stages of individuals belonging to the same spawning event (3 larvae stages, F and S seeds and parental adult tissues). Once genes are identified and fully annotated, differentially expressed genes between F and S seeds will be detected by mapping Hiseq-2000 platform data to the reference transcriptome and related metabolic pathways analysed. All this data will be used to create a microarray for use in future physiological experiments in order to gain insight into the molecular biology of growth.

Population dynamics in terrestrial slugs.

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KEY WORDS: Slug, Snail, Gastropoda Pulmonata.

Growth dynamics of wild populations of two pulmonate gastropods were researched along the year. Growth of the snail *Cornu aspersum* was studied from March 2003 to June 2004 in a population of Leioa (43° 19' N, 2° 59' W). On the other hand, growth of the slug *Arion vulgaris* was researched throughout its life-cycle from May 2010 to December 2011 in Kanala (43° 22' N, 2° 40' W).

Regarding the snail *Cornu aspersum*, each animal was ascribed to one of the five on-going age classes by analysis of shell features. Two additional sampling episodes (April 2003 and November 2003) were performed in order to measure individual metabolic expenditure at different temperatures. Recruitments occurred in spring and autumn, both of them succeeding to reach maturity in 11 months. Snails bigger than 15 mm hibernated from December to March. Smaller animals seemed to arouse earlier than bigger ones. Active growth was resumed after arousal and stopped in the aestivation period that occurred due to the unusually hot and dry summer of 2003.

The hibernation period is triggered by environmental factors such as photoperiod and temperature. However, snails smaller than 15 mm (i.e. less than 100 mg soft body dry weight) were unable to hibernate, remaining active throughout the whole winter. The metabolic rate of those small animals showed to be more thermodependent. Furthermore, their metabolic rate was related isometrically to the soft body dry weight, while bigger animals related allometrically ($b=0.6$). These results may tentatively be interpreted as indicative of a size threshold required to start storing the reserves needed to afford a long starving period like hibernation.

Concerning the slug *Arion vulgaris*, we have made clear that individuals in the Kanala population have a circannual life cycle. Egg hatching starts in early autumn and finishes at the end of winter. Maximal life weight is usually attained at the end of summer, just before the onset of reproduction. This slug is a semelparous species meaning that it reproduces only once in its lifetime.

We studied growth of slugs in Kanala in Urdaibai during 1994 and 1995 and, by means of a phenological approach and thanks to a financial support of our University, we have analyzed the same slug population in 2010 and 2011. Phenology is, according to Wikipedia, the study of periodic plant and animal life cycle events and how these are influenced by seasonal and interannual variations in climate.

We have modelled growth of slug by mean of several mathematical equations, so that critical events in the life cycle of slugs may be precisely dated and their confidence intervals quantified. Comparison of the parameters of the models shows that, apparently, hatching of slugs has occurred in 2010-2011 about four weeks earlier than in 1994-95. This value must be taken cautiously, because, according to Euskalmet, October of 2011 has been the driest and hottest in the last 30 years. As far as egg hatching is a temperature-dependent phenomenon, past year's four-week earliness in hatching may be the direct consequence of an exceptionally hot October.

From the parameters of the growth curves it may be deduced that maximal weight has attained 40 days later in 2010-11 than in 1994-95. It means that, in total, growth period of slugs in Kanala has extended for approximately two months and half. As far as maximal weight has not changed it may be interpreted that environmental temperature elevation may be increasing the metabolic rate of this poikilotherm.

Bacterial resistance to stress

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KEY WORDS: bacteria, adverse environments, resistance.

Prokaryotes have colonized all the habitats of our planet: air, soil, water, the human body (the inside and the corporal surface), etc. Their adaptation capacity and their physiological plasticity allow them to survive in habitats in which the environmental conditions are not the optimal ones for life. They are ubiquitous! They are the most successful biological group of the planet. This fact makes us think about the mechanisms they use to grow and survive in adverse conditions.

In our group we study three specific cases:

- a) How intestinal bacteria (*Escherichia coli*, *Enterococcus faecalis*, etc) survive in aquatic systems.
- b) How *Vibrio* survives in aquatic environments in which it has to resist variations in temperature outside its optimal growth range.
- c) How *Acinetobacter baumannii* survives in hospitals, where temperature, dryness and disinfectants are not optimal conditions for its growth.

Why have these three specific subjects attracted our interest?

- a) Human beings and animals are pathogenic bacterial reservoirs from which these bacteria reach aquatic systems through wastewater. So water works as a vehicle for pathogenic bacteria.
- b) *Vibrio* (i.e *V. cholerae*) has a maximum growth temperature at 28°C but it can survive in water in the cold season at 4°C, to exponentially grow again in the warm season (20°C), when the temperature increases. And with the increase in temperature that the climatic change implies, the seasonal distribution of *Vibrio* in water is modified.
- c) The ability of *A. baumannii* to survive in hospitals and in the above mentioned conditions has made this bacterium responsible for nosocomial infections.

We also propose an integrative question:

Do such different bacteria share any strategy that allows them to survive in non-optimal conditions for their growth?

Obviously, it is essential to use different kinds of methods and microbiological techniques for these studies. Our main work tools are, along with classical microbiological techniques:

- Epifluorescence microscopy
- Flow cytometry
- Fluorescence *in situ* hybridization (FISH)
- Proteomic profiles
- RNA profiling
- Molecular genetics approaches...
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Post-transcriptional mechanisms in bacteria and their regulation by environmental signals

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KEY WORDS: bacterial stress responses, antisense RNAs, degradosome, glycolysis

The ubiquitous presence of microorganisms is largely associated with their unique abilities to adapt and thrive in adverse environments. We use the Gram-negative bacterium *Escherichia coli* (*E. coli*) as a model organism to study post-transcriptional mechanisms controlling mRNA stability as well as regulation of these mechanisms by environmental signals. Our two major lines of research are briefly described below.

1. High-throughput screening and functional analysis of antisense RNAs with new roles in *Escherichia coli* stress responses

Recent studies revealed a new class of small antisense RNAs (sRNAs) that play important roles in regulatory mechanisms that enable *Escherichia coli* and other bacteria (including essential genera of pathogenic enterobacteria) to adapt to environmental stresses. Analysis of several stress-related sRNAs demonstrated that they can exert their regulatory functions by basepairing with their target mRNAs to alter mRNA translation and stability in an Hfq-dependent manner.

Given important functions of sRNAs in bacterial adaptation and virulence, the main goal of our project is to employ a combination of high-throughput biochemical, genetic and molecular biology approaches and characterize a large fraction of experimentally identified and *in silico* predicted sRNAs that have not been studied previously. The specific aims of the project are to

- (i) Characterize antisense RNAs with new roles in bacterial stress responses;
- (ii) Examine their regulatory functions using *Escherichia coli* as a model organism;
- (iii) Investigate how the formation of sRNA/mRNA complexes affect the fate of selected sRNAs and their targets, and determine the contribution of the RNA chaperone Hfq and cellular ribonucleases to the rate-limiting and subsequent steps in disassembly and processing of these complexes *in vivo*.

2. Analysis of protein-protein interactions and subcellular localization of glycolytic enzymes in *E. coli*

Previous work has shown that the glycolytic enzyme enolase is a major component of the degradosome, a multienzyme complex controlling RNA processing and decay in *Escherichia coli* (*E. coli*) and additionally containing RNase E, PNPase (exoribonuclease) and RhlB (DEAD-box helicase). While association of RNase E with RhlB and PNPase was shown to be critical for the normal efficiency of the degradosome-mediated RNA decay, the function(s) of enolase in the degradosome remains uncertain. As ATP is an important cofactor of the degradosome, the presence of enolase in this complex suggests that the degradosome-dependent RNA turnover and the enolase-mediated ATP production (glycolysis) may be coordinated through co-localization of both processes *in vivo*.

This assumption, in turn, raises a number of fundamental questions regarding the membrane organization of the glycolytic complex, its composition and interactions with the major components of the RNA degradosome. The long-term goal of our study is to perform in-depth analysis of the protein-protein network that control glycolysis and link this process to RNA turnover and sugar transport in *E. coli*. The specific aims of the project are to:

- (i) Identify interacting partners of glycolytic enzymes in *E. coli*;
- (ii) Reveal and validate specific protein-protein interactions involving glycolytic enzymes and their interacting partners and
- (iii) Test the contribution of these interactions to the subcellular localization and co-localization of glycolytic enzymes with the major components of the *E. coli* degradosome.

Application of omic technologies to study *Candida albicans* and *Scedosporium prolificans* fungal pathogenesis.

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KEY WORDS: Fungi, virulence, immune response.

The area of interest of our research group is the pathogenesis and virulence factors of two fungal types capable to produce diseases in human and animals. *C. albicans* is an opportunistic dimorphic fungus that causes numerous infections in immunosuppressed patients and *Scedosporium prolificans* is a fungus normally present in soil and environment but has been described as emerging pathogen because serious infections caused by this agent have been reported with increasing frequency in more recent years.

Research Fields in *Candida albicans*:

- **Proteomic analysis and Characterization of Antigen Determinants**

The identification of proteins expressed at different growth conditions and during differentiation is important to know the mechanisms that allow this fungus to become pathogenic. To do that the bidimensional electrophoresis and sequencing of proteins have been used.

By utilizing Western blot and Elisa techniques with human and animal sera we have performed the characterization of the molecules that stimulate the cellular immune response as well as humoral response and the activation of other physiological processes such as pro-inflammatory response and adhesion. The aim is to study these molecules in order to use them in diagnostic and therapeutic purposes.

- **Increase in tumor cell adhesion and metastasis**

We have demonstrated that whole cells of *Candida albicans* increased the metastasis in mice liver without induction of an infectious process. Fractionation of a yeast extract allowed us to characterize the molecules that trigger an increase in tumor cell adhesion to mouse hepatic endothelium. The aim of this study is to know the mechanism that enhances the adhesion and the molecules implicated.

- **Recombinant Proteins**

Pro-inflammatory and pro-tumoral effect: we are obtaining recombinant proteins that induce the activation of pro-inflammatory cytokines and an enhancement of the adhesion of tumor cells.

Research Fields in *Scedosporium prolificans*:

- **Proteomic Characterization**

We have established a protocol for the protein extraction of samples of this fungus, from both conidiospores and mycelia. We are building reference proteomic maps for this species by using IEF and 2D SDS-PAGE techniques. Moreover, we will characterize all the proteome of both morphologies using Shotgun proteomic sequencing to establish the protein differential expression related to morphologies and virulence.

- **Antigen Characterization**

We are analyzing the proteome of *S. prolificans* and searching antigens from this species using sera from human and preinfected rabbits as primary antibody.

Diagnosis

New molecular techniques are nowadays a powerful tool in diagnosis. We will use our acquired knowledge of the proteome of *S. prolificans* to produce a diagnostic kit for this species based on RT-PCR.

- **Detection of Antifungal Resistance-Related Proteins**

S. prolificans has been described as a natural multiresistant fungus. This inherent characteristic makes this fungus especially difficult to treat. A further study of the proteome under antifungal-stress conditions will permit us to identify the proteins and to describe the mechanisms involved in this complex resistance.

New approaches in genomics and molecular microbiology to detect *Aspergillus fumigatus* and *Salmonella enterica* in order to understand their infections

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KEY WORDS: *Salmonella enterica*, *Aspergillus fumigatus*, Epidemiology, Pathogenesis, Genomics, Proteomics, Gene expression, Detection, Diagnosis.

Our research group is responsible for research study of infections caused by different pathogens, both bacterial and fungal, their rapid detection and the study of their virulence factors. *Aspergillus fumigatus* is an opportunistic fungus able to cause a wide range of diseases, being invasive aspergillosis one of the most important with a high mortality. The lack of adequate diagnostic procedures leads to delayed treatments which increases the mortality of the infections. The pathogenicity of this fungus is polygenic and multifactorial and is not clear enough. The genome of the fungus has been sequenced but a lot of their proteins are hypothetical or with not clear functions. *Salmonella* is one of the leading causes of gastroenteric diseases, and typhoid fevers worldwide, mainly caused by products and derivatives of animal origin and water. Besides, new pathogenic variants of *Salmonella* have emerged in recent years, so a rapid and effective detection of the bacteria in these products is absolutely necessary. Our group has developed and patented methods for detection of the most frequent *Salmonella* serovars by multiplex-PCR, real-time PCR, and monoclonal antibodies.

OBJECTIVES

- Our goal is to go deeper into the knowledge of the molecular factors involved in the virulence of the fungus by analyzing the *A. fumigatus* transcriptome through the use of a whole genome microarray that we have developed
- In relation with our research with *Salmonella enterica*, our goal is to characterize molecularly emerging variants in order to determine their evolutionary origin and their epidemiology
- Finally, we focus on the discovery of new pathways involved in pathogenicity and virulence of these pathogens, useful for the development of methods for their rapid detection, control, and monitoring, or for the design of new therapeutic strategies

TECHNIQUES

- Conventional microbiological techniques for cultivation and detection of the microorganisms
- Development of animal models through intravenous and intranasal routes
- Systems for DNA and RNA extraction and stabilization; conventional PCR, real-time PCR, multiplex PCR, and RT²-PCR, and electrophoresis of these DNA and RNA; DNA sequencing
- Gene expression through the use of whole genome microarray hybridization, and Bioinformatics analysis
- Proteomic techniques and Protein sequencing
- Histological techniques

RELATIONSHIPS WITH RESEARCH CENTER AND ENTERPRISES

- Nacional Center for Microbiology, Instituto de Salud Carlos III, Majadahonda, Madrid
- University of South Carolina, Columbia, United States
- Laboratorios Bromatológicos Araba, Vitoria-Gasteiz
- Tecnalia, Vitoria-Gasteiz

GRANTS

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Marine microbes. Who are they and what do they do?

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KEY WORDS: marine microbe, function, diversity.

Our main objective is to unveil the dynamics of the microbial communities in the marine environment. We study the abundance, specific composition, diversity and function of the prokaryotes, bacteria and archaea, as well as of the bacterivorous protists. Our current research focuses on two projects:

The Project "**Circumnavigation Expedition Malaspina 2010; Global Change and Biodiversity Exploration of the Global Ocean**" (MICINN, CSD2008-00077). The Project Malaspina 2010 aims to 1) Evaluate the impact of global change on the ocean, 2) Explore the biodiversity of the deep ocean, 3) Analyze the repercussions of the expedition of Alejandro Malaspina, 4) Advance marine science in Spain and promote society's awareness of it, and 5) Train and attract young researchers to oceanography. Malaspina 2010 is an interdisciplinary Project with 7 thematic blocks (The Malaspina Expedition, Heat and Mass flow, Biogeochemistry, Optics and Phytoplankton, Contaminants, Zooplankton, and Microbial processes) and 4 transversal blocks (Dissemination, Training, Integration, and Coordination). The expedition, financed by the Spanish Ministry of Science, is made up of nearly 400 researchers from 19 Spanish institutions, and from the 16 associated foreign institutions which include NASA, the European Space Agency and the universities of California, Rio de Janeiro, Washington and Vienna. *In situ* measurements and sampling were carried out during 2010-11, and two research vessels were involved: the *Sarmiento de Gamboa* in the North Atlantic Ocean transect by 24 °LN, and the *BIO Hespérides* in a circumnavigation of the Earth (Cádiz-Rio de Janeiro-Cape Town-Perth-Sydney-Auckland-Honolulu-Panama-Cartagena de Indias-Cádiz). About 120.000 samples of water, air and plankton were taken from surface down to a depth of 5.000 metres, in 300 stations distributed over 42.000 nautical miles through the Atlantic, Indian and Pacific Oceans. The current research of the "**Microbial processes**" block aims to know the function of the microorganisms in biogeochemical processes, mainly transformations of organic matter, at the global scale, and to analyze the diversity of microbial communities, especially at high depths. Inside this block, our group is in charge of analyzing the hydrolytic enzyme activities of the bacterioplankton in the global ocean, with special focus on their distribution, kinetic behaviour, stability, and relationships with organic matter and with bacterial diversity. At present, the deep ocean is under-sampled, and therefore the analysis of microbial processes in these areas is of great importance.

The Project "**Cambio. Bacterioplankton Diversity and function of the bacterioplankton in the Eastern Cantabrian Sea: Grazing and nutrients as drivers of the seasonal change**" (MICINN, CTM2010-19308/MAR). This research Project focuses on 1) The specific composition and diversity of the bacterioplanktonic community in coastal waters of the Eastern Cantabrian Sea, 2) The identification of the seasonal changes in the relevant members of that community over multi-year time scale, 3) The establishment of links between the taxonomic diversity and the physiological function of bacterioplankton, resulting in an optimization of available resources, and 4) The relevance of protistan grazing, compared to other environmental factors, as a significant driver of the change of relevant members of the community. The results obtained in this Project will allow not only to generate baselines which will be essential references in future analysis of changing environmental conditions (anthropogenic global warming, acidification, toxic wastes, etc.), but also to achieve a higher predictive capability about the performance of the ecosystem under different seasonal conditions.

Entomology applied to Forensic research

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KEY WORDS: Arthropods, Forensics, Pest diagnosis and control, PMI estimation.

1.- Concept

Forensic Entomology applies the knowledge about the structure and dynamics of insect and other arthropods to assist in legal matters resolution, such as judicial (abuses, neglect, crimes or deaths) or economic problems (infestations or plagues), where the correct interpretation of the information provided by entomologic evidences can play a valuable or even crucial role, particularly, in Court proceedings.

2.- Applications

1. Evaluation of the insect activity in a sample to estimate
 - a. Postmortem Interval (PMI) in cases of murder, suicide or natural death.
 - b. Data, origin and type of contamination, abuses or neglects involved in myiasis of animals and dependent people (sick or elderly people and children), infestation of stored food, real property and other legal aspects.
2. Detection of toxics and/or drugs in corpse remains; bioaccumulation of chemical metabolites such as drugs in corpses and other remains.
3. Molecular identification of human cadavers, based on gut contents from entomological evidences.
4. Maggot therapy; larvae activity of some species can remove only the necrotic tissue and promote wounds healing.
5. Illegal traffic; the use of insects as geographic indicators provide information to solve illegal traffic of vehicles and goods deal.
6. Identification and estimation of damages to personal and other kind of properties.
7. Population control, to prevent sanitary and economics problems that some insects can cause (pest, disease vector, etc.)
8. Organic waste treatment, as the high metabolic activity of necrophagous species can be useful to reduce organic residues.

4.- Main Objectives that are being developed by the research group

1. To ensure common guidelines and standard protocols for best practice in forensic entomology that guarantee the collaboration with forensic pathologists and police.
2. To increase our knowledge about the necrophagous fauna in C.A.P.V.:
 - a) Morphological identification of the main infesting species.
 - b) Molecular tipification of the most relevant entomofauna for forensic purposes.
 - c) Estimate their developmental rates in our latitudes.
 - d) Establish the faunal succession patterns on cadavers in our biogeographical environment.
3. To develop different control strategies for the insect populations that cause damages in transported or stored feed, cattle, areal properties and other material damages.
4. To apply knowledge about developmental biology of necrophagous species suitable to an efficient waste management as a possible tool to reduce residues organic fraction.

Centre For Experimental Marine Biology and Biotechnology (Plentzia Marine Station): Biscay Bay Environmental Biospecimen Bank

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KEY WORDS: Plentzia Marine Station (PIE), Biospecimen Bank

CENTRE FOR EXPERIMENTAL MARINE BIOLOGY AND BIOTECHNOLOGY

The Experimental Marine Biology and Biotechnology Station (Plentzia Marine Station, PIE) is a research centre with a mission to provide science and biotechnology applications to sustain, protect, and restore coastal and marine ecosystems, with emphasis on links between environmental condition and the health of marine organisms and humans. PIE is equipped with state-of-the-art preparatory analytical instrumentation necessary to obtain high quality samples of environmental matrices that further will be used to identify and quantify pollutants and toxicants in the UPV/EHU general services; Level 3 biosecurity laboratories for dealing with viruses and other disease-causing organisms; safety aquaria for culture and experimentation with harmful algae; aquaculture facilities to produce/maintain selected marine species for research; mesocosms facilities, an environmental biospecimen bank; a genomic laboratory devoted to marine species, additional laboratories, offices, and spaces for students.

Research activities: identification of the effects produced by environmental pollutants (including metals, organic compounds, emerging substances and nanoparticles) and biological hazards (including toxins associated with harmful algal blooms) in the marine environment; diseases of marine organisms; use of aquatic organisms as experimental models to study human disease processes; effects of multiple stressors in coastal ecosystems; and toxicity testing and profiling for environmental risk assessment. PIE also will be devoted to elucidate the genomes of key marine species, the physiological and ecological contexts within which different traits are expressed, and the cellular and molecular mechanisms by which marine organisms deal with toxic materials, diseases, and other stressors.

THE BISCAY BAY ENVIRONMENTAL BIOSPECIMEN BANK

The Biscay Bay Environmental Biospecimen Bank (BBEBB), located within the PIE, will provide useful information about long-term variability and temporal trends in biota. Long-term variations in growth, reproduction, metabolic rates, etc., driven by global factors (e.g., oceanographical cycles and oscillations, climate change, large scale processes such as ocean acidification, etc.) may condition bioaccumulation and biological responses to pollutants and alter baseline values for environmental relevant parameters and may hence render any data on tissue concentration of pollutants in biota or on biological impact less valuable. Sections of BBEBB will be devoted to samples for biometry (e.g. mollusc shells or fish otoliths), reproduction (e.g. gonad tissue) or general biochemical/physiological condition determinations that will result very helpful to interpret pollutant levels, trends and toxicity. BBEBB is aimed to provide continuous updating of toxicity profiles and will include the following biological samples of target species (mussels, oysters, eels, grey mullets, anchovies, hakes -and other fish species-, slugs, earthworms ...):

- fixed and embedded (biopsies) for histopathology and immunochemistry
- lyophilisates for chemical analyses
- dried shells for biometric and chemical analyses
- cryogenized for molecular and cellular analysis (biomarkers, microarrays, ...)
- and a clone bank (toxicogenomics/proteomics/...) based on Genvault storage technology

Acknowledgements: PIE has been promoted by Bizkaiko Foru Aldundia/Diputación Foral de Bizkaia) and University of the Basque Country (UPV/EHU). Funding and support from Basque Government (IKERBASQUE, Education, University and Research Dept.), University of the Basque Country (Unit for Formation and Research, UFIPSE, UFI 11/37) and additional project sources (K-Egokitzen: ETORTEK Strategic Research Program; CBET Res Grp: Grant to Consolidated Research Groups, the Environment Department of the Biscay Government) are acknowledged.

Toxicity and mechanisms of action of metal nanoparticles.

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KEY WORDS: metal nanoparticles, toxicity and mechanisms of action, alternative methods, mussel, fish, environmental risk assessment.

In the last years, manufactured nanoparticles (NPs) are being incorporated in many consumer products, with domestic, medical, cosmetic, industrial and military uses. Concomitantly with the increasing applications for nanosized materials, concerns are growing because the properties of nanostructured materials and their potential input in ecosystems could lead to unknown health or environmental hazards. The idea that nanometer-scale particles behave differently from their bulk counterparts has led to propose a new category in the field of toxicology named nanotoxicology, which aims to assess the effects of these particles on living organisms.

Under the framework of the European NanoReTox project (The reactivity and toxicity of engineered NPs: risks to the environment and human health, CP-FP 214478-2) and the Spanish Nanocancer project (Determination of genotoxic and carcinogenic potential of metal NPs using alternative methods *in vitro* and *in vivo* with zebrafish and invertebrates, CTM2009-13477), the Consolidated Research Group "Cell Biology in Environmental Toxicology-CBET" of the Faculty of Science and Technology is assessing the toxicity of metal NPs using an integrated methodology in which alternative toxicity testing methods have special relevance. We evaluate the toxicity of metal NPs in comparison with the ionic and bulk forms of metals and, if present in the formulation, with the stabilising or surfactant additives. We employ three different experimental approaches in parallel:

1. ***In vivo* exposure of mussels *Mytilus galloprovincialis*.** Mussels, as an invertebrate species, are considered an alternative experimental model. Filter-feeding bivalves are potentially a target species of nanomaterials entering the water column and, thus, they are suitable sentinel species to monitor NP impact into the marine and estuarine environment.
2. ***In vitro* exposure of mussel cells.** Two different cell models, haemocytes and gill cells, are being used as representatives of the internal defence system and of epithelial cells in direct contact with water pollutants.
3. ***In vivo* exposure of zebrafish *Danio rerio*.** Zebrafish is an emergent experimental model in biomedicine. In this case, zebrafish are being exposed at two developmental stages: recently fertilised eggs up to the end of organogenesis (5 days) and juvenile-adult zebrafish.

In the three cases, a two-tier procedure is employed. A large set of NPs (CuO, TiO₂, Ag, Au, SiO₂, CdS and ZnO) at a wide range of concentrations depending on the expected toxicity is tested using different screening methods: short-term *in vivo* exposure of adult mussels or *in vitro* mussel cells to detect direct cytotoxicity and short-term exposure of zebrafish embryos. Based on the results of these experiments, in-deep studies are designed for selected NPs (CuO, Ag and CdS). In this second tier, longer-term exposures are run for mussels and adult zebrafish and a set of toxicity and bioaccumulation endpoints are assessed, while a battery of mechanistic assays are performed in the primary cell cultures. NP internalisation into cells was demonstrated by TEM and X-ray microanalysis. Oxidative stress appears to be one important mechanism to explain the toxicity of NPs such as CuO NPs and Ag NPs.

All results obtained up to date indicate that ionic forms are more toxic than nanoparticles and the latter are more toxic than their corresponding bulk forms. Ag NPs resulted the most toxic of metal NPs tested up to date. Some additives present in NP formulations show also significant toxicity and thus need to be considered in environmental risk assessment of NPs.

This work is also supported by grants to Consolidated Research Groups (GIC07/26-IT-393-07), UFI11/37, and PhD fellowships (UPV/EHU).

Enzyme and Cell Technology

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KEY WORDS: enzyme, biocatalysis, microalgae, cyanobacteria, magnetic nanoparticles, cross-linked enzyme aggregates (CLEAS), endostatin, chiral hydroxyalkanoic acids, biodiesel, bioethanol, biosurfactants, CO₂ sink, added-value products.

The main goal of the Enzyme and Cell Technology Group is the **use and development of nanotechnologies** which employ **biocatalysts** (isolated enzymes or microbial cells) for **industrial, environmental or biomedical applications**. The Group has experience and equipments for the production, purification and characterization of proteins and enzymes with industrial or biomedical interest. For this purpose there are available techniques to culture heterotrophic (bacteria, yeasts and fungi) and phototrophic (eukaryotic microalgae and cyanobacteria) microbial cells in orbital incubators or bioreactors (fermentors and photobioreactors). Also there are available technologies for the immobilization of biocatalysts by adsorption or covalent-linking onto solid supports, and entrapment in polymeric matrices which allows their use in reactors of different design and operation modes at laboratory scale.

Recently, other nanotechnologies have been developed for the synthesis and functionalization of magnetic nanoparticles with enzymes or cross-linked enzyme aggregates (CLEAS) of interest in industrial biotechnology and biomedicine. Thus, lipases have been immobilized to catalyze the transesterification reactions to produce biodiesel and biosurfactants as well as polyhydroxyalkanoate depolymerases, enzymes capable to degrade bioplastics in order to obtain chiral monomers for the synthesis of bioactive compounds of interest in pharmacy or other functionalized bioplastics. Also intensive cultures of microalgae in helicoidal photobioreactors showing remarkably tolerance to CO₂ are being investigated as components of new biological CO₂ sinks of utility to mitigate the release to the atmosphere of industrial gas effluents. The resulting cell biomass will be evaluated as a source of biotechnological added-value products and of reserve oils or polysaccharides of interest to produce biodiesel or bioethanol, respectively.

Among the available analytical or preparative techniques are remarkable the use of VIS/UV spectrophotometry, preparative (LPLC y FPLC) and analytical (HPLC) chromatographies, and electrophoresis (isoelectrofocussing, native PAGE, SDS-PAGE, 2D-PAGE) for the separation and characterization of proteins and nucleic acids. Moreover, the Group possesses facilities and experience to carry out techniques for protein isolation and characterization, enzyme assays, protein cross-linking, image analysis, and the design and operation of lab-bench bioreactors and photobioreactors. Also molecular biology techniques for gene cloning, PCR, and for the expression, purification and characterization of recombinant proteins are available.

At present, the on-going **basic** and **applied** projects are:

- Recombinant human endostatin derivatives: a tool to improve protein stability and to study protein-protein interactions
- Enzymic degradation of bioplastics for producing chiral monomers
- Enzyme expression in thermophilic cyanobacteria
- Synthesis and functionalization of magnetic nanoparticles with enzymes and cross-linked enzyme aggregates (CLEAS) to obtain biodiesel and biosurfactants
- Utilization of microalgae as a CO₂ sink and as a source to obtain biofuels and other added-value products
- Catalysis of ester-forming reactions in non-aqueous media to synthesize biodegradable polymers

These researches were funded by grants from UPV/EHU, the Basque Government (SAIOTEK), MICINN, MSC, Instituto de Salud Carlos III and the European Union.

Biomembranes and their role in new therapeutic strategies search.

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KEY WORDS: Drug targets, bacterial conjugation, bacterial biofilms, modified oligonucleotides.

Membranes define the external boundaries of cells and regulate the molecular traffic across that boundary. Not only the lipidic composition and its organization but also the presence of some specific proteins and the regulation of traffic across it are crucial for well functioning of the cell. Because of that, the membranes are at the origin of a great number of diseases. Moreover, drug administration depends on the traffic across the membrane. Taking into account these facts, it can be deduced that biological membranes are crucial for the development of both new drugs and new strategies for drug delivery. Our research group studies different processes that happen at the membrane level and that are related to different health problems. We believe that the study of those processes at the molecular level will shed light on the treatment by identifying new drug targets or by developing new drug delivery systems.

1. **Bacterial Conjugation.** Bacterial conjugation provides the transfer genetic material among bacteria and is responsible of the spread of antibiotic resistance among pathogenic bacteria, which constitutes a major public health burden. It requires direct contact between both bacteria and therefore the membrane plays a crucial role. Our research group has studied TrwB, a membrane protein that plays an essential role in bacterial conjugation of plasmid R388. We have determined that the transmembrane domain of TrwB plays a regulatory role in its biological activity. Therefore, the transmembrane domain, could be a therapeutic target for controlling the spread of antibiotic resistance. In this regard, since T4CPs are key elements of conjugative process, it seems necessary to identify other T4CPs to study their properties to find a common molecular pattern among them. Our research group focuses now on studying other T4CPs to develop novel therapeutic strategies to counter chronic infections by inhibiting the activity of T4CPs.
2. **Bacterial biofilms.** Bacterial biofilms are involved in most of the chronic infections and since they are extremely resistant to antimicrobials, they represent a real health problem. In this regard, it has been suggested that the connection between conjugation and biofilms may influence the chances of biofilm-related infection risks. In this regard, our group is developing a transversal strategy of research: i) analysis of the membrane proteomic profile of biofilms to narrow the spectrum of targets aimed to control biofilm formation and ii) study of the bacterial conjugation process in biofilms, in particular the molecular mechanisms of key proteins like T4CP. This combined approach could shed light on the new therapeutic drugs, other than antibiotics, to develop. To accomplish this aim drug libraries and high-throughput technology are being used.
3. **Conjugated nucleotides.** We are also interested in process where the traffic across the membrane is the key step. In particular, in the internalization routes of oligonucleotides inside eukaryotic cells. This work has been focused particularly on the study of the conjugation approach analyzing different modified oligodeoxynucleotides in order to test targeted delivery and enhancement of cellular permeability. The first objective has been based on the investigation of cellular uptake profiles of glucose-DNA conjugates with different carbohydrate presentation in two different cell lines which have cell-surface carbohydrate receptors. The second goal has been undertaken by the use of lipid-DNA conjugates with different alkyl chain presentation. The main interest of this project lies in the possibility of improving the formulation of siRNAs with sugars or lipids to increase their effectiveness as drugs in gene therapy.

LIPID METABOLISM AND SIGNALING GROUP

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KEY WORDS: ceramide 1-phosphate, sphingolipids, apoptosis, inflammation, migration, cancer

Background: cell and tissue homeostasis is essential for regular development of an organism. When this is altered, metabolic dysfunctions and disease are prone to occur. Therefore, the maintenance of an appropriate balance in the activation / inhibition of the different metabolic pathways and cell signaling systems is fundamental for normal cell physiology. Although enzymes, and proteins in general, have been considered the major players for regulation of cell biology, lipids are not less important. Among the different bioactive lipids, sphingolipids are of particular importance. This lipid class has classically been considered to be the building blocks of cell architecture. However, extensive research over the last two decades has clearly established that some sphingolipids, including ceramide, sphingosine, and their phosphorylated forms ceramide 1-phosphate (C1P) and sphingosine 1-phosphate (S1P), are bioactive and can regulate essential biological functions. Specifically, these metabolites regulate signal transduction pathways that are involved in angiogenesis, apoptosis, cell proliferation, differentiation, intracellular trafficking, migration, senescence, inflammation and cancer.

Research interest: our laboratory is interested in the control of inflammation and tumorigenesis by sphingolipids. Specifically, we are focused on the elucidation of the mechanisms by which bioactive sphingolipids control cell migration, growth and survival of immune and tumor cells.

Selected recent publications:

P. Gangoiti, M. H. Granado, L. Arana, A. Ouro, and A. Gómez-Muñoz. "Activation of protein kinase C is essential for stimulation of cell proliferation by ceramide 1-phosphate". *FEBS Lett.* 584, 517-524 (2010)

L. Arana, P. Gangoiti, M. H. Granado, , A. Ouro, and A. Gómez-Muñoz. "Ceramide and Ceramide 1-phosphate in health and disease". *Lipids Health Dis.* 5, 9-15 (2010)

P. Gangoiti, L. Camacho, L. Arana, A. Ouro, M.H. Granado, J. Casas, G. Fabriás, A. Gómez-Muñoz. "Control of metabolism and signaling of bioactive sphingolipids". *Prog. Lipid Res.* 49, 316-334 (2010)

A. Gómez-Muñoz, P. Gangoiti, M. H. Granado, A. Ouro, and L. Arana. "Ceramide 1-phosphate in cell survival and inflammatory signaling". *Sphingolipids as signal and regulatory molecules. Adv Exp Med Biol.* 688, 118-30 (2010)

P. Gangoiti, L. Arana, A. Ouro, M. H. Granado, M. Trueba, and A. Gómez-Muñoz. "Activation of mTOR and RhoA is a major mechanism by which ceramide 1-phosphate stimulates macrophage proliferation". *Cell. Signal.* 23, 27-34 (2011)

L. Arana, P. Gangoiti, A. Ouro, I-G. Rivera, M. Ordoñez, M. Trueba, R.S. Lankalapalli, R. Bittman, and A. Gómez-Muñoz. "Generation of reactive oxygen species (ROS) is a key factor for stimulation of macrophage proliferation by ceramide 1-phosphate". *Exp. Cell Res.* 318, 350-360 (2012).

Protein folding and the role of molecular chaperones

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KEY WORDS: chaperones, Hsp 40, Hsp70, Hsp100, nucleoplasmin, chromatin remodeling

Living systems host a crowd of molecular chaperones that act with different mechanisms and serve to maintain protein homeostasis. Our group studies nuclear and cytosolic chaperones. Among the cytosolic chaperones we are interested in members of the Hsp60, Hsp70 and Hsp100 families. In particular, we are analysing the functional cycle of these proteins and how they interact with substrates and modulate their conformation. We are also trying to understand how Hsp70 and Hsp100 proteins collaborate, forming a productive network, to disaggregate and refold cellular protein aggregates. Among nuclear chaperones we focus on nucleoplasmin (NP), a histone-chaperone involved in the exchange of basic proteins bound to DNA that regulates, for instance, the sperm chromatin remodeling during the fertilization process and the chromatin changes at the onset of embryogenesis in *Xenopus*. Our studies have characterized different nucleoplasmin-histone complexes to understand the role played by nucleoplasmin in the chromatin remodeling processes. These studies are carried out using a combination of biochemical (expression and purification of proteins, mutagenesis, hybrid oligomeric proteins) and biophysical (fluorescence, IR spectroscopy, calorimetry, circular dichroism, ..) techniques.

References:

"Nucleoplasmin binds histone H2A-H2B dimers through its distal face". I. Ramos, J. Martín-Benito, R. Finn, L. Bretaña, K. Aloria, J.M. Arizmendi, J. Ausió, A. Muga, J.M. Valpuesta, A. Prado. *J Biol. Chem.* 285, 33771-33778 (2010).

"Role of DnaJ G/F-rich domain in conformational recognition and binding of protein substrates". J. Perales-Calvo, A. Muga and F. Moro. *J. Biol. Chem.* 285, 34231-34239 (2010).

"Energetics of nucleotide-induced DnaK conformational states". S.G. Taneva, F. Moro, A. Velázquez-Campoy and A. Muga. *Biochemistry* 49, 1338-1345 (2010).

"Allosteric communication between the nucleotide binding domains of caseinolytic peptidase B", J.A. Fernández-Higuero, S.P. Acebrón, S.G. Taneva, U. del Castillo, F. Moro, A. Muga. *J. Biol. Chem.* 286, 25547-25555 (2011).



Matematika/Matemáticas

Foliation theory

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KEY WORDS: foliated space, lamination, singular Riemannian foliation, noncommutative geometry.

Our research consists of the dynamic, metric and cohomological study of *foliated spaces*, and the analytic and K-theoretical study of the corresponding noncommutative spaces.

Nowadays, foliation theory is a multidisciplinary field, essentially non distinguishable from *dynamical systems theory*. It involves several and complex geometric, topologic, analytic and measurable techniques. In the last decades, the specialists in the subject have developed new fruitful research lines by removing some of the restrictions imposed to *classical foliated manifolds*. In particular, our group focuses its work in:

- 1) the study of some types of *singular foliations* (removing the *regularity conditions*);
- 2) the analysis of some *laminations* (elimination of *transverse differentiability*) and of some topological or measurable *pseudogroups* provided with simplicial structures (suppression of *tangential differentiability*);
- 3) the examination of *generic properties* in a topological and measurable sense (elimination of *totality hypothesis*);
- 4) the *noncommutative study (à la Connes)* of some foliated spaces (deletion of *commutativity*).

Foliation theory is playing and will play a fundamental role in the qualitative study of both the physical (cosmology and solid state physics) and the biological world (molecular biology, genomics and evolution), and appears increasingly in other science fields.

Our concrete objectives can be classified in two main blocks:

- 1) *The study of metric and dynamical properties of foliated spaces* and its relations. Tilings and repetitive graphs give us examples of minimal laminations, useful in the testing of properties and relations. Moreover, noncommutative geometry gives topological and measurable tools that allow us to complete this study (see [1], [2], [3] and [4]).
- 2) *Cohomological study of singular Riemannian foliations*. If we classify the points following the different dimensions of the leaves, we obtain a stratification of the main manifold. We study the relation between the *basic cohomology* and the cohomology of the ambient manifold, through algebraic tools such as exact sequences and spectral sequences (see [5] and [6]).

Last publications:

[1] F. Alcalde Cuesta, P. González Sequeiros y Á. Lozano Rojo, *Affability of Euclidean tilings*. C. R. Acad. Sci. Paris, Ser. I 347 (2009) 947-952.

[2] F. Alcalde Cuesta, Á. Lozano Rojo y M. Macho Stadler. *Dynamique transverse de la lamination de Ghys-Kenyon*. Astérisque 323 (2009) 1-16.

[3] F. Alcalde Cuesta, Á. Lozano Rojo y M. Macho Stadler, *Transversely Cantor laminations as inverse limits*. Proceedings of the AMS 139 7 (2011) 2615-2630.

[4] Á. Lozano Rojo, *An example of non-uniquely ergodic lamination*. Ergod. Th. & Dynam. Sys. 31 2 (2011) 449-457.

[5] J.I. Royo Prieto, M. Saralegi y R.Wolak, *Tautness for riemannian foliations on non-compact manifolds*, Manuscripta Math. 126 (2008) 177-200.

[6] J.I. Royo Prieto, M. Saralegi y R.Wolak, *Cohomological tautness for Riemannian foliations*, Russian Journal of Mathematical Physics. 16 3 (2009) 450-466.

Mixed Integer Stochastic Optimization: Algorithms and Applications.

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KEY WORDS: stochastic, multistage, optimization, risk, CPLEX, COIN-OR.

Stochastic Optimization is currently one of the most robust tools for decision making. It is broadly used in real-world applications in a wide range of problems such as finance, scheduling, production planning, industrial engineering, capacity allocation, energy, air traffic, logistics, etc. The uncertainty, that is inherent to most of the problems, can be modeled via a scenario tree, which represents the possible future realizations of the uncertain parameters. The Determinist Equivalent Model (DEM) can be expressed by a compact or a splitting variable representation. We have designed the break stage scenario clustering for scenario partition that considers an alternative representation of the DEM. It is given by a mixture of the compact representation into the scenario clusters and the splitting representation between them.

We have developed an exact algorithmic framework for optimizing large-scale mixed integer multistage stochastic problems, so called BFC-MS. The experimental C++ code uses the optimizer IBM ILOG CPLEX and the open Computational Infrastructure for Operations Research COIN-OR. It has been tested in randomly generated instances and real-life problems. In particular, the proposed approach has been implemented for solving a Natural Gas Network Transportation Infrastructure provided by the Norges Teknisk Naturvitenskapelige Universitet (NTNU, Trondheim, Norway). The problem consider a high volatile demand a long a time horizon of 4 years, and has been modeled with 1000 scenarios, almost a hundred thousand of constraints, more than 34 thousand 0-1 variables and more than 22 thousand continuous variables. These are big dimensions for plain use of today state-of-the-art optimization engines such as FICO XPRESS and CPLEX, since those engines could not solve the problem in an affordable elapsed time. The Branch-and-Fix Coordination Methodology developed has obtained the solution in 182 seconds. Additionally, we have analyzed the advantages and disadvantages of using Lagrangean bounds and its specialization for our algorithms. We are using the Lagrangeans for bounding purposes in the branching candidate so-called Twin Node Families over a set of scenario clusters for obtaining the optimal solution for some of the auxiliary submodels in several steps of the BFC algorithms. We have worked on different Lagrange multipliers updating schemes as the Subgradient, Volume Algorithm, Progressive Hedging Algorithm, and Dynamic Constrained Cutting Plane scheme. Also, the experimental C++ code uses the optimizer CPLEX within COIN-OR. Decomposition Benders approach requires to appending feasibility and/or optimality cuts to the master problem until the iterative procedure reaches the optimal solution. The cuts are identified by solving the auxiliary submodels attached to the scenarios. Cluster Benders Decomposition (CBD) based scheme allows to identify tighter feasibility and optimality cuts in reasonable computing time.

The stochastic optimization models consider, in general, the optimization of the objective function expected value alone (so, the neutral risk environment is assumed). It is not a bad practice assuming that the variance of the objective function over the scenarios is small. However, there are some approaches that additionally deal with risk measures in the more realistic risk aversion environment. These measures consider semi-deviations, excess probabilities, conditional value-at-risk and stochastic dominance as risk measure-based functions to optimize. Those approaches are more amenable than the classical mean-variance schemes. In this sense, we will study the risk aversion strategies in the applications, as well as the impact to introduce them in the BFC algorithms.

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2012 mathematical technology transfer

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KEY WORDS: high order finite element simulations, rostering, scheduling, image processing, electric demand, mathematical modelling.

A "mathematical model" can be defined as a formal description of a real world phenomena. Such models are very useful, since they enable calculations and therefore quantitative predictions concerning the behaviour of the considered phenomena. Additionally, mathematical modelling enables to run simulations that aim to improve designs and establish strategies to direct a given process under study towards the desired objective.

A particular example of this consists of the simulation and design of several engineering devices such as various waveguides needed in communication satellites. In our group, we have employed high-order finite element methods to simulate these waveguides and improve their design.

We have also worked in the field of Image Processing and Computer Vision, where variational models have a special interest. With this modelization technique, the problem we want to solve is posed in terms of the minimization of an energy functional in integral form. The numerical solution of this minimization process requires advanced techniques of optimization and partial differential equations, such as the Level Set Method.

Among the great variety of problems that can be stated in a variational formulation, we can find image segmentation (i.e., the decomposition of an image into regions corresponding to distinct objects), the merging of 2D views of a scene into a 3D model, image restoration, super-resolution (enhancement of the resolution through the combination of different views of the same scene), and so on. The fields of application include medical imaging and video-surveillance.

We also work on optimisation and operational research, which aims at finding the best solution to a problem involving different types of variables that must meet predetermined conditions. They can be described in short as "the science of what is best". They can be applied to numerous problems, and more applications are emerging day by day as a result of the need for decision-making in many areas where new models need to be formulated and new algorithms developed to reach adequate solutions.

An other area of work has to do with the introduction of wind power that is limited by its dependence on the weather and the difficulty of storing the surplus for use in times of low production. One way to attack this problem is to move from a system based on electricity production that responds to the unpredictable caprices of demand, to other where the consumption is adapted to production.

The team that we present here has broad experience in collaborations with companies in the fields mentioned above. Specifically, we have conducted projects and contracts with INKOA Soluciones Agroalimentarias, Sidenor I+D, Metro Bilbao, Cespa, Fundación Aguas de Barcelona, EuskoTren, Ferrocarriles de Vía Estrecha (FEVE), Cementos Pórtland Valderrivas, Eroski S. Coop and Tecnalia Research & Innovation among others.

<http://www.ehu.es/mae/grupottm/>
<https://sites.google.com/site/numemagroup/>

Biostatistikako Ikerketa Taldea.

Grupo de Investigación en Bioestadística

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KEY WORDS: Biostatistics; Clinical research; Transfer

The main specific objectives of the group are to detect problems of scientific interest in the biomedical and experimental fields where biostatistics can contribute to their resolution; conduct our own research in biostatistics aimed at generating results for solving the problems; create necessary computer tools and software for its implementation; and apply the proposed methods to the considered problems, helping to interpret the results and draw final conclusions, in collaboration with biomedical and experimental researchers involved.

Other objectives of the group are basically transversal, such as, to give methodological support in biostatistics to other research groups in the fields of biomedicine or experimental sciences; to promote the transfer of the research done at the university in biostatistics to biomedical and experimental fields; to take advantage of the strong demand for support in biostatistics to detect future research in this area, that respond to real problems in other fields.

ACTUAL RESEARCH TOPICS:

1. **Categorization of continuous clinical variables.** In daily clinical practice physicians encourage statisticians to categorize continuous variables. We propose a methodology to categorize continuous variables based on Generalized Additive Models with *P-spline* smoothers. We graphically display the relationship between the continuous covariate and the response variable and we look for the optimal cut-off points based on different criteria.
2. **Dealing with missing data in medical studies.** Medical research studies based on follow-up measurements are often subject to high rates of missingness. Many researchers use different imputation methods, such as simple imputation methods (mean, regression imputation, K-Nearest Neighbours (KNN)) as well as more advanced methods (e.g., MCMC Multiple Imputation), to avoid losing valuable information. We work on the selection of the appropriate imputation method in each case
3. **Item Response Theory analysis applied to Health Related Quality of Life (HRQoL) instruments.** The goal is to extend the psychometric evaluation of HRQoL instruments using the Item Response Theory (IRT). We applied the proposed IRT to the Health Related Quality of Life in Eating Disorders-sort form (HeRQoLED-R) questionnaire in a new sample of patients to obtain greater precision in the estimation of parameters and increase its validity.
4. **Propensity Score.** We use the propensity score to reduce the confusion by matching. The propensity score is the conditional probability receiving a treatment depending on some factors. It is calculated using logistic regression, where the dependent variable is the treatment. The propensity score is used as a matching technique. The most common use is the nearest neighbour methods.

FOR MORE INFORMATION LOOK AT THE FOLLOWING WEB PAGE

<https://sites.google.com/site/biostit/>

Matrix Analysis and Applications Group

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KEY WORDS: Matrix Analysis, Control Theory, Linear Systems, Invariants, Perturbation

The aim of our research is to gain knowledge of mathematical problems that arise in the development of Control Theory. The methods to be used run over almost all fields of mathematics: from linear algebra and matrix analysis or combinatorics to differential geometry or commutative algebra. More specifically, the goals can be divided into three categories:

- a) Structural properties of linear and piecewise-linear control systems.
- b) Geometry and parametrization of the solutions of several problems in control theory.
- c) Change of the invariants when matrices and systems are perturbed or deformed.

In particular, for the next three-year term we will focus on the following aspects of these problems according to the two main research lines of the group:

1. Mathematical Control Theory:

- Search for canonical forms and systems of invariants of bimodal systems as well as for linear systems under restricted feedback equivalence.
- Study of the invariants appearing in the solutions of some important control problems as well as their characterization and assignability.
- Study the geometry and topology of the solutions of the generalized partial realization problem and the controlled invariant subspaces of bimodal systems.

2. Perturbation Theory:

- Characterization of the admissible feedback invariants by perturbing the control matrix of a linear system.
- Study of quantitative problems on spectral perturbation of matrices.

Weekly seminars are held where the progressive work of the group members are shown, the difficulties are discussed, other researchers' work related to our problems is explained. A joint research project is shared with a group of Universidad Politécnica de Cataluña. Annual meetings are held to keep track of the advances on the project.

More information in: <http://www.mae.ehu.es/s0100-gigamhom/es/>.

GRECA: Groups, Representations and Algebraic Combinatorics

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KEY WORDS: Groups, Characters, Algebraic Combinatorics.

The frame of our research is Group Theory and Representation Theory and their applications to Algebraic Combinatorics. Our **main lines** of interest are the following:

1. **Finite p-groups.** We study the power structure and conjugacy classes of elements and subgroups.
2. **Pro-p groups.** The problems on the power structure of finite p-groups translate naturally to pro-p groups. We are also interested in their co(homology) and on some questions related to functions defined by words.
3. **Characters.** We try to see how some properties of the characters (degrees, zeroes, fields of values...) reflect or are reflected in the group structure. In a different direction, we study the characters of some important families of p-groups.
4. **Algebraic Combinatorics.** We work in the construction of some objects of combinatorial nature (t -designs, difference sets, association schemes,...) using algebraic techniques.

Mathematical Analysis and Applications. Mathematical Physics

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KEY WORDS: Partial Differential Equations, The Dirac equation, Helmholtz equation, Null-Control and measurable sets.

We study different partial differential equations that have played a fundamental role in various areas of modern physics and mathematics. Those equations are the Dirac equation, Helmholtz equation and the Heat equation.

The Dirac Equation:

The free Dirac equation describes a relativistic electron or positron which moves freely as if there were no external fields or other particles. We are interested in studying how electromagnetic forces have influence on it. On the one hand, the property of being self-adjoint is a fundamental information to study operators in quantum mechanics. Therefore we see that the Dirac operator with an Hermitian matrix potential that has a Coulomb type singularity is self-adjoint. On the other hand, the 3D Dirac equation can be listed as a dispersive equation. It is interesting to quantify dispersive phenomena for the perturbed flows by using Strichartz estimates. However, those estimates fail for some potentials. We construct some counterexamples to Strichartz estimates for the magnetic Dirac equation.

Electromagnetic Helmholtz equation:

The Helmholtz equation is an elliptic second order partial differential equation which is encountered in many branches of mathematical physics as in the theory of elasticity or theory of electromagnetic waves. In order to solve this equation uniquely, there must be additional restrictions on the behavior of the solution at infinity. These restrictions are the so-called Sommerfeld radiation conditions.

We study the Helmholtz equation with magnetic (vector) and electric (scalar) potential that describes the interaction of a free particle with an external electromagnetic field. Under suitable assumptions on them, we prove that there exists a unique solution of this equation satisfying some a priori estimates and Sommerfeld radiation conditions that allow us to deduce some applications to the corresponding evolution equation and the scattering theory associated to it.

Null-Control and measurable sets:

The control for evolution equations aims to drive the solution to a prescribed state starting from a certain initial condition. One acts on the equation through a source term, a so-called distributed control, or through a boundary condition. To achieve general results one wishes for the control to only act in part of the domain or its boundary and to have as much latitude as possible in the choice of the control region: location, size, shape. We prove the interior and boundary null-controllability of some parabolic evolutions with controls acting over measurable sets.

Mathematical Analysis and Applications. Numerical Analysis

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KEY WORDS: Numerical Analysis, Partial Differential Equations, Computational Methods, Stochastic Differential Equations, Hermite Spectral Methods.

Numerical Schemes for the mKdV Equation:

The family of partial differential equations related to the Korteweg-de Vries is a well known pattern used to modelize several physical processes as the motion of the curvature of some geometric flux, the vortex patch, ferromagnetic vortices, fluid mechanics, traffic models, anharmonic lattices, hyperbolic surfaces, etc. The goal of this work is the design of numerical schemes that approximate the solutions of the initial value problem and that are robust for long time simulations. We take advantage of the fact that these equations preserve an infinite number of conservation laws in order to choose the schemes that incorporate some discrete invariants has the norm or the energy. Finite difference methods as well as pseudo-spectral methods have been used for approximating the solutions and we conclude that the second ones are more efficient, presumably due to the oscillatory nature of the solutions.

Numerical Simulation of the N-Dimensional Sine-Gordon Equation via Operational Matrices:

We develop a numerical method for the N -dimensional sine-Gordon equation using differentiation matrices, in the theoretical frame of matrix differential equations. Our method avoids calculating exponential matrices, is very intuitive and easy to express, and can be implemented without toilin any number of spatial dimensions. Although there is currently a vast literature on the numerical treatment of the one-dimensional sine-Gordon equation, the references for the two-dimensional case are much sparser, and virtually nonexistent for higher dimensions.

A Mean Extinction-Time Estimate for a Stochastic Lotka-Volterra Model:

We study a stochastic Lotka-Volterra model; we prove the nonnegative character of its solutions for the corresponding backward Kolmogorov differential equation; we propose a finite element method, and finally, we make a direct comparison between predictions and numerical simulations of stochastic differential equations (SDEs).

Hermite Spectral Methods:

When numerically approximating the solution of a partial differential equation posed in an unbounded domain, an alternative to the truncation of the domain is the use of a family of functions defined in this unbounded domain as the orthogonal basis for spectral methods. Hermite functions are orthogonal in the whole real line with respect to an exponential weight. We have defined Galerkin and collocation Hermite spectral approximations to the solutions of scalar linear hyperbolic equations posed in the real line, and proved spectral convergence rate of both approximations under certain assumptions on the coefficients of the equation.

Probability and Applications Group

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KEY WORDS: Probability, Bernstein-type Operators, Inequalities, Stochastic Orders, Classification.

The aim of the group's research is twofold. On the one hand, to get deep into the interesting connections between probability theory and other branches of mathematics, such as approximation by positive linear operators, analytical inequalities or combinatorics. On the other hand, we apply these interrelated techniques to various areas of statistics and applied probability, such as reliability theory, actuarial sciences or biometrics.

- Approximation by Bernstein-type operators. Bernstein-type operators are constructed as mathematical expectations and this fact allows the use of resources of probability theory to investigate many of their properties. Our contribution, in collaboration with another group from the University of Zaragoza, has consisted in the consolidation of these probabilistic techniques by obtaining many new interesting results on convergence, preservation of shape properties, best constant, ... some of which are difficult to deal with, or even inaccessible by means of the usual analytical methods.
- Analytical inequalities. The probabilistic approach of some classical analytical inequalities, like Ostrowski inequality and Hermite-Hadamard inequalities, has led us to obtain results that generalize and present in a unified way most specific results founded in the literature.
- Combinatorics. Many combinatorial sequences are, at the same time, sequences of moments of probability distributions. Our main aim is to characterize the sequences for which this phenomenon occurs and find a satisfactory explanation of it.
- Stochastic orders and related hypothesis test. The mainly aim is to develop a duality theory between some stochastic orders coming from economics and reliability theory and the relationships satisfied by the mean order statistics of two ordered variables. This theory would be of both theoretical and practical interest. In particular, we have solved various testing problems involving stochastic orders assumptions and having applications to different fields such as economics, reliability theory and biology.
- Supervised classification. If we make random observations in several groups, the aim of the supervised classification is to obtain a classification rule that allows to assign a new observation to some of the groups. These problems came from a famous work by Fisher in 1938 and have a lot of applications in many different fields. We have tried to extend Fisher's rule to situations in which there is no homocedasticity or the dimension of the data set is too big.



Geologia/Geología

Coastal Geology

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KEY WORDS: Atlantic coast, environmental transformation, natural processes, anthropogenic impact, sea-level changes

The Coastal Geology research group (www.ehu.es/harea-geologicalitoral) develops a multidisciplinary approach (sedimentology, geochemistry, micropalaeontology, topography, radiometric chronology) to characterize natural and anthropogenic processes responsible for the environmental transformation of the coastal zone during the last climate cycle (Holocene and Anthropocene). Its different activities can be summarized into the following research lines and recent publications:

1. **Environmental transformation of polluted and regenerated ecosystems.** The coastal area has experienced an intense human pressure that provoked its continuous physical destruction and a deep chemical and biological transformation. The development of environmental conservation and regeneration schemes on particular ecosystems makes necessary to carry out geological studies in order to evaluate their modern characteristics, their historical alteration processes, and the feasibility of environmental improvement proposals/ Cearreta, A.; García-Artola, A.; Leorri, E.; Irabien, M.J. & Masque, P., 2012, Recent environmental evolution of regenerated salt marshes in the southern Bay of Biscay: anthropogenic evidences in their sedimentary record, *Journal of Marine Systems*.

2. **Sea-level variations as a consequence of anthropogenic climate change.** An increase in the sea-level rise rate is potentially one of the most devastating impacts of the future climate change on the coastal areas. Climate change influences the coastline at decadal and centennial scales, and these variations of the relative sea level are registered in the coastal sedimentary sequences. The combined study of historical records and high resolution geological reconstructions of the relative sea level is a powerful tool/ Leorri, E.; Cearreta, A. & Milne, G., 2012, Field observations and modelling of Holocene sea-level changes in the southern Bay of Biscay: implication for understanding current rates of relative sea-level change and vertical land motion along the Atlantic coast of SW Europe, *Quaternary Science Reviews*.

3. **Holocene environmental evolution due to natural processes.** Due to the frequent, rapid and intense climate changes that characterize the late Quaternary period, coastal environments have experienced dramatic variations and contain a very complete record of the processes and events occurred during this time interval. The high-resolution multiproxy study of this sedimentary record allows to reconstruct the past features, to understand the present conditions and to deduce the possible future environmental variability/ Alday, M.; Cearreta, A.; Freitas, M.C. & Andrade, C., 2012, Modern and late Holocene foraminiferal record of restricted environmental conditions in the Albufeira lagoon, SW Portugal, *Geologica Acta*.

4. **Sedimentary processes with social and economic consequences.** Sedimentary processes in the estuarine areas are frequently altered by man-induced activities which can lead to undesirable repercussions. Sedimentological studies contribute to understand the role of the anthropogenic influence and to establish suitable strategies for sustainable development/ Monge, M., Cearreta, A. & Evans, G., 2012, Morphodynamic consequences of dredging/dumping activities along the lower Oka estuary (Urdaibai Biosphere Reserve, southeastern Bay of Biscay, Spain), *Ocean and Coastal Management*.

5. **Geological assessment of archaeological deposits.** Human exploitation of natural resources has left a significant footprint in the environment since ancient times. Evaluation of pollution levels and ecological impacts derived from these historical activities in archaeological deposits is possible/ Irabien, M.J.; Cearreta, A. & Urteaga, M., 2012, Historical signature of Roman mining activities in the Bidasoa estuary (Basque Country, northern Spain): an integrated micropalaeontological, geochemical and archaeological approach, *Journal of Archaeological Science*.

The Coastal Geology group has a leading role in the Postgraduate Programmes (Master and Doctorate) and the recently created UFI on Quaternary: Environmental Changes and Human Footprint (www.mastercuaternario.ehu.es).

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Palaeogene Working Group: Global Boundary Stratotype Section and Points (GSSPs) of the Palaeogene in the Basque Coast

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KEY WORDS: Cretaceous, Palaeogene, Stratigraphy, Micropalaeontology.

The history of the Earth, since its formation about 4600 million years ago, has been punctuated by several events, most of which are recorded in the rocks that make up the planet. Geologists investigate these events "reading" the information stored in the rocky materials that crop up in different places of the Earth's surface. The ultimate goal of this knowledge is to be able to predict the consequence of similar events that may happen again in the future. To this end a referential Geological Time Scale must be constructed first. This scale is a valid global frame divided into intervals (Eons, Eras, Periods, Epochs and Stages) whose definition is based primarily on Stratigraphy, i.e., the study and interpretation of strata or layers of rocks formed by the accumulation of sediments. The International Commission on Stratigraphy (ICS) is responsible for selecting the geological sections worldwide that best represent the boundaries between unit intervals, i.e., the stages. Stage boundaries are defined by Global Stratotype Sections and Points (GSSPs).

Our group has organized several international meetings in 2006, 2007 and 2009, which showed the international community, and ultimately the ICS, the high geological quality of the Basque coastal cliffs. These are a worldwide reference to observe and study sedimentary rocks accumulated in deep-marine settings during the geological time that extends from the Early Cretaceous to the Eocene, a lapse interspersed with some of the most significant global change events.

- The Cretaceous/Tertiary boundary interval is recorded in the Aitzgorri headland at Zumaia and in the Sopelana beach, reference sections of deep-marine deposits worldwide. In addition to an iridium-rich clay layer, a complete record of the various palaeontological events that typify the transition between the two geological periods has been obtained, as well as of several magnetic polarity reversals. Furthermore, the Cretaceous/Tertiary transition at Zumaia shows spectacular, well-exposed sedimentary cyclicities that were forced by orbital fluctuations of the Earth during that time interval.
- The Danian/Selandian and Selandian/Thanetian boundaries are recorded in the Itzurun beach at Zumaia and in the Sopelana beach. The Itzurun beach was selected as the stratotype section for the Danian/Selandian and Selandian/Thanetian boundaries. This section contains the most complete and best-preserved record worldwide, mainly in terms of the succession of marine plankton events, polarity reversals of the Earth's magnetic field and orbital Milankovitch cycles for both boundaries.
- The Palaeocene/Eocene boundary interval is recorded in the Itzurun beach at Zumaia, a world-class reference section for the study of this boundary in deep-marine deposits. A prominent global warming or hyperthermal event occurred during this interval, characterized by rapid temperature increase and a major extinction of deep-sea benthic foraminifers, probably caused by a massive release of greenhouse gases. Past episodes of greenhouse warming provide insight into the coupling of climate and the carbon cycle and thus may help to predict the consequences of unabated carbon emissions in the future, including the ecosystem response and evolution.
- The Ypresian/Lutetian Working Group of the ICS resolved, during a Workshop held in Getxo in September 2009, to define the stratotype for the base of the Lutetian stage in the Gorrondatxe beach section (Getxo), at approximately 47,8 million years ago. This section contains the most complete and best-preserved record worldwide of the succession of marine plankton events, polarity reversals of the Earth's magnetic field and orbital Milankovitch cycles. The proposal was ratified by the International Union of Geological Sciences in April 2011, and the "golden spike" placed in Gorrondatxe in February 2012.

Palaeogene Working Group: Lines of research of the Upper Cretaceous and Paleogene in the Basque-Cantabrian Basin and the Betic External Zones

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KEY WORDS: Cretaceous, Palaeogene, Stratigraphy, Micropalaeontology.

The research group, composed of palaeontologists and sedimentologists, has been active since 1988. Over these 24 years the research of the group has been focused on the study of the Upper Cretaceous and Lower Palaeogene successions from two complementary viewpoints: Micropalaeontology (biostratigraphy and palaeoecology) based on planktonic foraminifers and calcareous nannofossils; and Stratigraphy and Sedimentology of continental, shallow-marine and deep-marine facies.

Our research has mainly centred on the Pyrenees, exactly in the area known as the Basque-Cantabrian Basin, and the Betic External Zones. In addition, sections from Tunisia, Egypt and México have also been studied.

Our particular research lines are the following:

- Palaeoclimatic-palaeoceanographic record: analysis of global climate-change events in the Palaeogene and implications for the behaviour of the present day geo-biosphere.
- Hydrocarbon reservoir models: architecture and evolution of carbonate and siliciclastic sedimentary systems.
- Marine communities and ecosystems in the Palaeogene: structure, diversity, biostratigraphy and evolution.
- Chronostratigraphy of the Palaeogene.

Among the most significant results achieved to date, the following are worth highlighting:

- (a) A notable improvement in the reconstruction of the stratigraphic architecture and of the palaeogeographic evolution of the western Pyrenees (Basque-Cantabrian Basin).
- (b) A more precise bio-, chrono and magnetostratigraphic zonation of the sedimentary succession, mainly at the Cretaceous-Tertiary boundary, the lower Palaeocene (Danian *sensu lato*), the Palaeocene-Eocene boundary and the Ypresian-Lutetian boundary.
- (c) A better understanding of the influence of tectonism, sea-level changes and climate changes on continental and marine sedimentation.

Members of the group take part in projects focused on the development of a general model for macroporosity related to ancient platform margin karst systems (Lower Palaeogene successions of the Urbasa and Andia ridges in Navarre).

Finally, this research group has been involved in projects that aimed to spread the social awareness of the value of geological features included in the landscape, providing knowledge and technical consultancy to the management institutions of, for example, the Ordesa and Monte Perdido National Park and the recently established Protected Biotope of the coastal transect from Deba to Zumaia, so that they can use this geological information in their twofold protectionist and pedagogic duties.

The services that the group can provide are summarized as follows:

- Theoretical-practical training in sedimentary basin analysis; advice to carry out geological mapping
- Analysis of current sediment dynamics
- Climate records: Palaeoclimatology
- Biostratigraphic and palaeoenvironmental studies
- Micropalaeontological application for resource prospecting
- Assessment of the conservation of the geological and palaeontological heritage and of its recreational and educational use and management

Vertebrate faunas from the Mesozoic and Cenozoic of the Basque-Cantabrian Region and adjacent areas. Taphonomy, palaeobiology and palaeontological heritage. Collaboration program between the UPV/EHU, the Centre National de la Recherche Scientifique (CNRS) and the Muséum National d'Histoire Naturelle (MNHN, Paris).

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KEY WORDS: Vertebrates, Mesozoic, Cenozoic, Taphonomy, Palaeobiology, Palaeontological Heritage, Iberian Peninsula.

A collaboration program that involves researchers from the Universidad del País Vasco/Euskal Herriko Unibertsitatea (UPV/EHU), the Centre National de la Recherche Scientifique (CNRS) and the Muséum National d'Histoire Naturelle of Paris (MNHN) was signed in 2007 and has been renewed in 2010 for three years.

The main aim of this research collaboration is the study of the vertebrate fossil remains from the Mesozoic and Cenozoic of the Basque-Cantabrian Region and adjacent sedimentary basins of the Iberian Peninsula. Taphonomical, palaeobiological and biochronological aspects are considered. The vertebrate faunas are compared to other contemporaneous assemblages, mainly from fossil collections (such as those preserved in the Muséum National d'Histoire Naturelle of Paris, France). Moreover, this collaboration contributes to a recognition of the value of the palaeontological heritage and the conservation of the studied vertebrate sites.

The main research topics are as follows:

- Continental and marine vertebrates from the Late Cretaceous of the Basque-Cantabrian Region (in collaboration with J.C. Corral, Museo de Ciencias Naturales de Álava/Arabako Natur Zientzien Museoa, Vitoria-Gasteiz).
- Marine reptiles from the Jurassic of the Asturian Basin (in collaboration with J.C. García-Ramos, L. Piñuela and J.I. Ruiz-Omeñaca, all from the Museo del Jurásico de Asturias - MUJA, Colunga).
- Marine mammals and turtles from the Paleogene of the Pyrenean basins (in collaboration, among others, with J.I. Canudo and G. Cuenca, Grupo Aragosaurus-IUCA, Universidad de Zaragoza).
- Study of microvertebrate faunas from the Late Quaternary of the Cantabrian Range.

Main contributions and results:

- Description of the most complete plesiosaur specimen found in Spain, one of the very few juvenile plesiosaurs known worldwide, from the Liassic rocks (Pliensbachian) of Asturias (Bardet et al., 2008, *J. Vert. Paleontol.*).
- First occurrence of the sawfish *Onchosaurus* in the Iberian Peninsula on the basis of a tooth from the Late Cretaceous (Coniacian) of Burgos (Corral et al., 2012, *J. Vert. Paleontol.*).
- Discovery of a skull fragment with teeth of the mosasaurid *Prognathodon* cf. *sectorius* from the Late Cretaceous (Campanian) of Navarre (Bardet et al., 2012, *Bull. Soc. Geól. France*).
- Description of new sirenian (sea cow) remains from the Middle Eocene (Lutetian) of Navarre (Astibia et al., 2010, *Geol. Mag.*), and study of the histological features of the ribs (Buffrénil et al., 2008, *Geodiversitas*). These and other sirenian remains found in the Middle Eocene of Huesca (Badiola et al., in prep.) are the oldest reported from Western Europe.
- Description of a new species of the "zhelestid" mammal *Lainodon* from the Late Cretaceous (Campanian) of the Laño Quarry in the Condado de Treviño (Gheerbrant & Astibia, in press; *Bull. Soc. Geól. France*). An update of the continental and marine vertebrates from the Campanian-Maastrichtian of the Laño Quarry is currently in progress.

Support provided by the Ministerio de Ciencia e Innovación (research projects CGL2007-64061/BTE and CGL2010-18851/BTE) and by the Gobierno Vasco/Eusko Jaurlaritz (research groups CGL07/14-361 and IT-320-10).

Mass transfers through the lithosphere

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KEY WORDS: lithosphere, delamination, tectonics, structural geology, transpression, extensional collapse.

Our main research topics are the mass transfers in the continental crust, a key point for the dynamics of the lithosphere. The most important processes of mass transfer through the lithosphere are due to the motion of ductile shear zones and the intrusion of huge volumes of igneous rocks. They are mainly concerned with the links between the intrusion of plutonic rocks and the nucleation and development of ductile shear zones.

We integrate field studies of Structural Geology, rock fabric analyses, measurements of the anisotropy of the magnetic susceptibility and gravity data in order to perform 3-D models. Since this approach is concerned with geological processes rather than with regional questions, we have selected a few working areas which encompass the main steps of a complete orogenic cycle:

- **Oceanic subduction** in La Puna and the Eastern Cordillera (Salta, NW Argentina), with special emphasis on the Calama-Olapato-El Toro lineament, representing a transfer zone associated to an important change in the subduction angle of the Nazca plate below the South America plate. Magmatism, recent volcanism and active seismicity related to mantle delamination of the South American plate can be also tested in this area.
- **Continental collision and transpression**, in the Central-Iberian Zone of the Iberian Variscan belt and in the central and western Pyrenees. In the Pyrenees the study analyses the evolution from continental collision to transpression during the Hercynian orogeny (Benasque and Panticosa sectors) and the superposition of the Alpine orogeny. In the Central-Iberian Zone we are mainly working in the internal structure and emplacement of granite plutons, as a way to test the influence of lithospheric delamination in old orogens.
- **Extensional collapse**, in Betic Cordilleras. The interest of this area is due to the presence of the Ronda peridotites, the largest outcrops of the subcontinental mantle in the world, which allows a unique chance to analyse the deformation of the lithospheric mantle at the Earth's surface.

All of these areas are suitable to test melt-enhanced deformation processes related to the interplay between shear zones and igneous melts. The members of the applying institutions, Universidad del País Vasco and Salamanca in Spain and CONICET in Argentina, have the methodological and regional expertise required for this type of works. The results of this research represent a significant advance in the knowledge of both, the emplacement of granite plutons and the rheological behaviour of rocks during the nucleation, kinematics and evolution of ductile shear zones. These are essential factors for the geodynamic interpretation of orogenic belts.

Molecular-level structured materials for energy and mass exchange and storage

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KEY WORDS: Microporous materials, MOF, SOFC, Batteries, nanodevices, applications, catalysis, energy.

The design of new materials can be tackled from diverse perspectives, and the most recent advances are determined by the possibility of providing applicability to the chemical compounds from the lowest structural level which defines them as such; this is, from the crystal structure itself. [Adams, J., Pendlebury, D., Global Research Report, Evidence, UK, 2011] The latest results in an extension of the classic concept of a material, from the macroscopic level down to the tiny field of the molecular entities.

The development of clean-energy generation systems is one of the greatest challenges that can be tackled from this approach. In this area, the most promising devices are the fuel cells, which allow the conversion of the chemical energy into electrical energy and heat. Our research team has worked in the optimization of cathode materials for SOFCs following a strategy that includes the design and the definition of the composition and also the microstructural improvement of the materials. In addition, an interlayer between the cathode and the electrolyte has been developed and optimized to prevent the reactivity between them. In SOFC technology is necessary to point out that, in spite of the made advances, the marketing of these systems needs still a lot of work of research focused principally on increasing the lifetime of the cells. These systems of energy generation demand parallel scientific challenges, without which their final application would not be viable.

Another approach for the energy efficient management is the development of the required materials for rechargeable batteries. The efforts of the scientific community have been focused on obtaining and development of cathodes based on Li^+ ion. However, alternative systems with Na^+ , Ca^{2+} and Mg^{2+} cations, fundamentally, have been also studied. Another important aspect related to the electrochemical properties of the cathodes is the particle morphology and size. These properties can be changed varying the preparation conditions, and also by further thermal and mechanical processing. Different compounds susceptible to have ionic conductivity have been obtained in our research group.

The mass storage and transport represents a second approach to the issue, because it leads the question to the need of porous materials. In this sense, the possibility to store gaseous fuels deserves special mention. Additionally, the devices for *in situ* processing of waste products should be also mentioned. The porosity also implies the existence of larger surface areas that makes these materials potentially applicable in catalytic processes. The combination of porosity together with other interesting physical and chemical properties allows obtaining multifunctional materials with potential applications in asymmetric catalysis, enantioselective separation, and electronic sensor devices. Our research team has a deep background in the synthesis and study of inorganic-organic materials, templated and coordinated, as well as in coordination polymers. The coordination polymers are considered the most promising materials for the storage, adsorption and separation of gases and molecules of different nature, in catalysis and other bioapplications. Sometimes, these materials can be functionalized pre- and post-synthetically maintaining the original crystal structure.

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**Fisika-Ingeniaritza Elektronikoa/
Física-Ingeniería Electrónica**

RF and Microwave Group

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KEY WORDS: high frequency electronics, power amplifiers, noise characterization, radio-communication systems.

The main goal of our group is the development of novel techniques for the analysis, design and characterization of power amplifiers and full front-ends in the RF and microwave domain.

The increasing complexity of communication signals impose a severe R&D effort focused on new device technologies, new design techniques, advanced analysis and simulation strategies and innovative and rigorous experimental characterizations. In particular, power amplification is currently one of the main bottlenecks to achieve the strict performances of RF transmitters for modern applications. Power amplifiers are, in a great extend, the main responsible for DC consumption of the transmitter and for signal intermodulation distortion. Consequently, power amplifier design is a critical step that has to be carefully studied as a function of the application in order to obtain an acceptable compromise between linearity and efficiency. Our group has developed an extensive work on analysis and characterization of power amplifiers, including circuit linearization, circuit modeling and system simulation. We maintain fruitful cooperation with other laboratories and international institutions. As an example, we can mention the advancements on spurious oscillation detection in power amplifiers achieved in the framework of a project funded by the French Space Agency (CNES, Toulouse, France) in cooperation with Thales Alenia Space (TAS-F). Our group has also a relevant activity in noise characterization of RF circuits and systems, where it is worth mentioning the development of novel techniques for the amplitude noise and phase-noise measurement in the presence of large-signal excitations. Finally, we develop today intense activity on RF instrumentation for particle linear accelerators (LINACs).

Epidemic models: Vaccination strategies based on impulsive control techniques with, potentially, gain-scheduling and adaptive inter-vaccination periods.

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KEY WORDS: Epidemic Models, Control Theory, Vaccination Strategies, Impulsive Control.

Control Theory allows focusing on a large variety of different problems if one is able to identify the manipulated variables which can be potentially used as controls. This research deals with the synthesis of vaccination strategies based on control techniques with the main objective of eradicating the propagation of an epidemic disease. A mathematical model for the propagation of the disease in the population is required before the synthesis of any vaccination strategy in a Control Theory context. In this sense, epidemic models are of nonlinear differential or discrete equations and in general, they can be formulated as dynamic systems. The most used models in the literature are:

- SI models where the population is divided in susceptible to the infection (S) and infectious (I)
- SIR models where a removed-by-immunity population (R) is added to the SI model
- SEIR models which distinguishes between infected population without external symptoms, called exposed population (E), and those with external symptoms, called infectious population (I)
- SVEIR models which incorporates a vaccinated population (V) to the SEIR model

The sub-populations in such models are the state-variables of the dynamic system. All of such models can be subject to the application of a vaccination strategy in order to achieve the main control objective, i.e., the eradication of the epidemic disease from the population. In this context, several control techniques coming from the Control Theory can be considered for such a purpose. In summary, the main strategies to be used are:

- A regular vaccination being either constant or time-varying. In the later case, the vaccination may be based on state-variables feedback control techniques, with potential addition of a state-observer to estimate online the values of the state-variables if their true values are not available.
- An impulsive vaccination based on the application of vaccines during short time periods. This kind of vaccination campaigns can be mathematically described by means of impulse functions. In this context, the impulse magnitude may be constant at all impulse time instants or time-varying. Moreover, the impulse time instants may be uniformly distributed in time or not. Then, such possibilities give place to consider alternative ways of designing the vaccination strategy.
- A vaccination strategy combining the aforementioned ones, i.e., a regular vaccination combined with an impulsive one. Furthermore, prediction techniques via a discrete reformulation of the models on a fixed side planning horizon, or of varying size, may be incorporated to adjust the impulses amplitude and the inter-vaccination periods.
- Vaccination strategies based on the technique of the exact input-output linearization via a state-variables feedback control law. Such a control technique issues a linear closed-loop system from a nonlinear one, as it is any of the epidemic models under our study. Moreover, the parameterization of the control law allows place the poles of the closed-loop system at desired locations. In this way, the control designer can choose appropriately such control parameters in order to achieve the main objectives.

Research group on Experimental Automatic Control: GAUDEE

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KEY WORDS: Control, nanopositioning, smart materials, mechatronics, active magnetic bearing, vibration control

The Experimental Automatic Control Group of the department of Electricity and Electronics, GAUDEE, is a group of teachers and researchers in the field of Systems Engineering and Automatic Control that focus its activity on the development and application of advanced control techniques, combining both basic science and applied science and technology. The group is interested in solving questions of importance in production or industrial processes. It is involved in several research projects like smart materials, magnetic levitation systems and the control of large scientific facilities (in collaboration with ESS-Bilbao).

NANOPOSITIONING WITH SMART MATERIALS

Smart materials are capable of responding, in a controlled fashion, to one or more different external stimuli. External stimuli can be physical or chemical, like magnetic or electric fields, and the response can, for example, be a change in dimensions. There are a large number of applications of these materials as sensors or actuators, especially when trying to reduce their size.

Ferromagnetic shape memory alloys (FSMAs) are a particular example of smart materials. They exhibit large strains (-6%) under applied magnetic fields, meaning they don't need to be directly contacted to be actuated. However, the hysteretic nature of the material presents a challenge to the control of the material, and requires a purpose-built controller.

From this line of research, we propose different actuator prototypes based on FSMAs and several strategies to control them. A home-built actuator, a commercial one and new actuator based on two orthogonal fields are controlled. So far, very encouraging results have been obtained and positioning accuracies on the order of nanometers are achieved.

A new line of research for the group is the development of a displacement sensor with nanometric resolution based on high frequency resonant cavities.

VIBRATION CONTROL OF ROTATING MACHINERY SUPPORTED BY ACTIVE MAGNETIC BEARINGS

The use of active magnetic bearings (AMBs) for supporting the spindle in rotating machines provides a large number of remarkable advantages over conventional bearings. The lack of physical contact eliminates the need of lubrication, makes possible very high rotational speeds and results in longer life for the mechanical components. However, due to the unstable nature of the AMBs, it is necessary to include a control loop to stabilize the system. The increasing complexity of the closed-loop system can be balanced by introducing an additional control action for active suppression of the different vibrations that can appear in the shaft.

In a first stage, the main research activities have been related with the accurate modeling and position control of the whole system (spindle+AMBs), taken into account the coupling due to the gyroscopic effect, the vibrations caused by the unbalance or the nonlinearities in the magnetic force. In particular, different strategies have been proposed to attenuate the vibrations induced in the shaft during rotation due to the unbalance. Recently, within the European project DYNXPERS, the group is involved in the development of a high performance spindle head. Two main objectives are considered: Calibration and Chatter avoidance. The active magnetic bearings are used to calibrate the system under changes of the tool or working conditions and to detect the appearing of the chatter instability during the machining. Further, control strategies are being developed to improve the damping when the chatter is predicted.

RF and Control Applications for Particle Accelerators

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KEY WORDS: RF instrumentation and control, beam diagnostics, particle accelerators, EPICS.

Researchers from the RF and Microwave, and the Automatic Control Group of the Department of Electricity and Electronics collaborate with ESS Bilbao in the development of RF and Control Applications for Particle Accelerators, being an important part of such activities performed in locals of the Faculty of Science and Technology (UPV/EHU). The research activities refer to problems, both from basic science and from applied science and technology in the field of Particle Accelerators, where RF and control play a relevant role. The activities include the development of beam diagnostics, RF devices and controls, and the corresponding electronics.

EPICS AND DISTRIBUTED CONTROL SYSTEMS

EPICS is a set of Open Source software tools, libraries and applications developed collaboratively and used worldwide to create distributed soft real-time control systems for scientific instruments such as a particle accelerators, telescopes and other large scientific experiments. Goals of the group using EPICS:

- To integrate modern control standards in a single system for scientific installations together with usual tools of the automatic controls.
- To develop this middleware to get an efficient and secure communication between all devices, redistributing messages and requests.
- To compare different EPICS developments and solutions, using hardware testbenches.
- Particle Accelerators and EPICS. The research group is involved in the integration of some diagnostics and control devices (BPMs, LLRF) usual in the field of Particle Accelerators into an EPICS net.

PARTICLE ACCELERATOR SCIENCE

The group is involved in several developments for particle accelerators, in particular, for the ESS Bilbao proton LINAC. Among these it is worth mentioning:

- Beam diagnostics and related electronics: active projects are related with Beam Position Monitors, which allow to determine the beam bunches position with very high precision; the integration between EPICS and the RF Cavities control system, which is a key issue in the diagnostics and control area; and SEM grids, a beam profile diagnostic based on secondary electron emission.
- ISHN and ISHP Projects: The objective is to develop and test two type of hydrogen ion sources (H^+ , H^-) using a similar beam diagnostics setup. The project includes the control and diagnostics systems of the whole facility and it is leaded by ESS-Bilbao, in collaboration with several facilities like the pulsed neutron and muon source ISIS (Oxfordshire UK). Several entities have participated in the construction, the companies AVS, Elytt Energy and Jema Group, Tekniker-IK4 research centre, among others.

RF INSTRUMENTATION AND CONTROL

In an RF LINAC, the particles are accelerated by a RF signal with an appropriate amplitude and phase, through a high power transmission chain with a wide range of control systems.

The research group is collaborating with the ESS-Bilbao team on:

- Low-Level RF controls of frequency, amplitude and phase of accelerating RF signals injected into the particle accelerating structures and to get linear and spurious-free behavior of RF transmitters
- RF subsystems for Beam Position Monitors and other Diagnostics
- RF subsystems to optimize RF signal injection in RF cavities for plasma generation or particle acceleration
- Experimental characterization and conditioning of low and high power RF devices and subsystems

RF applicator and biocompatible Fe₃O₄ nanoparticles for magnetic hyperthermia.

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KEY WORDS: magnetite nanoparticles, superparamagnetism, hyperthermia.

Iron oxides nanoparticles have acquired great relevance in the area of biomedical diagnostics and therapy. Among many others they include magnetic separation, magnetic resonance imaging (MRI) contrast agents, targeted drug delivery or magnetic hyperthermia. The principle of magnetic hyperthermia is based on the exothermic properties of magnetic materials under the influence of an alternating current magnetic field. Magnetic particles interact with the field and dissipate energy to their surroundings. It has been shown that tumor cells are more sensitive to heat compared to healthy cell. Therefore, magnetic hyperthermia is a promising cancer thermotherapy. Taking into account these facts chemists, physicists and physicians form the NANOBIOTERM multidisciplinary team to develop functionalized nanoparticles with the aim of applying them in hyperthermia.

The main objective of the research is the localized thermal ablation of malignant tumours in the liver using magnetic nanoparticles.

For this purpose, the first step is the production and characterization of biocompatible nanoparticles, which must present an hydrophilic surface. Nanoparticles have been obtained directly by aqueous or organic based synthetic procedures. In aqueous solution nanoparticles with low crystallinity, low saturation magnetization and broad size distribution are usually obtained. Preparations in organic media render nanoparticles surrounded by a shell of hydrophobic ligand molecules, which provide control over the size, crystallinity and shape of nanoparticles. In this last case, nanoparticles must be converted into water soluble ones and for this purpose we have used the incorporation of an amphiphilic polymer.

The second step has been to optimize the quantity of nanoparticles that must be inoculated in the tumors in order to be monitored by magnetic resonance imaging (MRI). For evaluating the hepatic distribution MRI was performed in healthy animals.

The next step in this research was the development of liver cancer tumours in a group of rats and the inoculation of the magnetic nanoparticles to study the expected reinforced selectivity of the functionalized nanoparticles to the malignant tissue. It has been demonstrated that different concentrations of magnetite are delivered to the liver metastasis depending on the degree of evolution of the tumor. MRI has shown that magnetofluid concentrates in early developed metastasis. This fact has been corroborated by ICP measurements of iron in liver after injections.

Finally, SAR values of the nanoparticles have been calculated from the heating curve obtained by heating a known mass of nanoparticles. The SAR value is defined as the thermal power dissipation per unit mass of the nanoparticles. Different SAR values have been obtained by measuring the synthesized magnetite NPs in different alternating magnetic fields ranging from 0.1 to 0.9 MHz and from 6 to 10 kA/m. The values increase with the intensity of the magnetic field, although they are lower than those obtained in related materials, which could be explained because of the particle size, size distribution and measurements condition.

In the nearly future, nanoparticles targeted with specific ligands which can recognize superexpressed molecules appearing in angiogenesis will be synthesized. The optimization of the synthesis conditions must be performed in order to improve size distribution to obtain better hyperthermia SAR values.

ACKNOWLEDGMENT

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Microstructural, magnetic and spectroscopic characterization of materials with high technological applications

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KEY WORDS: Magnetic Nanoparticles, Fe-Al Intermetallics, Semiconductors Optoelectronics, MSMA

The group is comprised of seven members of two different departments that master magnetic and spectroscopic (Mössbauer, Photoluminescence and Positron Annihilation) techniques. They carry out the following research lines:

-Magnetic nanoparticles (NPs) and the development of a new cancer therapy. Magnetic noble metals have become a reality in the XXI century. Our research group has been able to synthesize Au, Ag and Cu magnetic NPs, surrounded by organics elements and has demonstrated for the first time, that the origin of magnetism present in the gold NPs reside only in Au atoms on the surface of the NPs. We have extended it to another non-magnetic materials in bulk like to pure ZnO, who's NPs, synthesized by us, show a magnetic behaviour too.

Our group is developing, within a disciplinary team, the cancer therapy called magnetic hyperthermia (ablation of cancerous tissue by means of magnetic NPs). Indeed, we have already built several prototypes of electromagnetic applicators for magnetic hyperthermia and the last one can work in the frequency range 100-1000 KHz at applied magnetic fields up to 15 kA/m over volumes high enough to insert laboratory rats.

-Magnetic shape memory materials for use in magnetic controllers-actuators capable of working at high frequencies without external temperature variation. We are working in this line with the purpose of determining the influence of atomic disorder on their properties, and particularly the influence of vacancy-type defects on them.

-Fe-Al based intermetallic alloys in order to understand the influence of different parameters on the complex magnetic behaviour of these intermetallics in ordered and deformed alloys.

-Compound semiconductors for optoelectronic applications, where we are currently focused on the study of ZnO because of its great potential in device applications in the region ultraviolet-blue. Our objective is to characterize the optical properties of ZnO crystals and heavily doped ZnO (bulk material and heterostructures) grown by different methods in order to identify the defects responsible for their luminescent properties.

-Polymeric materials for electrical insulators, where we are studying the aging process of these materials in order to prevent their failure in service. The knowledge of the physical processes, which control the electrical and mechanical stability of polymers during in-service ageing, is critical to predict the long-term lifetime of these components.

-Early cancer detection. This is a research line we have started very recently in collaboration with researches of the BIO fundation to compare the different electronic structure of healthy and neoplastic tissues in order to try to develop a technique for early cancer detection.

The work above has been carried out under different financial assistance from various agencies and institutions.

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Software Technologies Working Group (GTTS, <http://gtts.ehu.es>)

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KEY WORDS: Information Retrieval for Multimedia Resources, Language and Speaker Recognition/Verification, Automatic Speech Transcription, Automatic Video Subtitling/Captioning

Research at GTTS focuses on fundamental software technologies, in particular those related to speech processing and information retrieval. We are working on speech segmentation, language and speaker recognition/verification, speaker diarization, automatic speech transcription, video subtitling, etc. Part of our efforts are devoted to develop tools and prototypes for various applications:

1. The spoken document retrieval system (Hearch: <http://gtts.ehu.es/Hearch/>) which looks like a conventional search tool (such as Google, Bing, etc) but is designed to retrieve audio/video segments based on the automatic transcription of speech contents (broadcast news repositories in Spanish and Basque).
2. The automatic bilingual video subtitling applied on the plenary sessions videos that the Basque Parliament posts in its website (<http://www.parlamentovasco.euskolegebiltzarra.org/>), running from September 2010.

Finally, we also devote great efforts to academic training (doctoral thesis and master), dissemination of results (both in prestigious publications and through technology transfer to companies in our area) and collaboration with other research groups.

ACTIVE PROJECTS

- Spanish MICINN under national plan of R+D+I, 2010-2012 (TIN2009-07556): Search and access to the information contained in the speech of multimedia resources.
- Saiotek (Basque Government), 2011-2012 (S-PE11UN065): Detection and identification of speakers in different audio signals: meetings, TV broadcast and telephone conversations.
- University-Society (UPV/EHU and Basque parliament), 2012-2013 (US11/06): Search platform of multimedia contents for business and scientific exploitation.

RESEARCH ACTIVITY IN THE LAST FIVE YEARS

- UPV/EHU Research Group: 2011-2013 (50.000 euro)
- Projects and contracts: 13 (470.000 euro)
- Publications: 35 (4 journals, 31 peer-reviewed conferences)
- Thesis: 2 presented and 2 in progress
- Participation in international competitions:
 1. NIST Language Recognition Evaluation (2007, 2009 and 2011)
 2. NIST Speaker Recognition Evaluation (2008 and 2010)
- Organization: the Albayzin 2008 and 2010 Language Recognition Evaluations (in collaboration with the Spanish Thematic Network in Speech Technologies)

TECHNOLOGY TRANSFER

- Hitzaldi: tool for audio-text alignment in parliamentary interventions.
- Sautrela: software package (free access) for the development of speech processing applications.
- Hearch: search tool for audiovisual resources (from automatic transcriptions of speech)
- Kalaka and Kalaka-2: databases for the development of language recognition systems.
- ICT- COST 278: database of TV news in Spanish and Basque for audio segmentation and speaker diarization.

Electronic and optical excitations in nanostructures

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KEY WORDS: nanostructure, nanocontact, overlayer, quantum well state, plasmon, DFT, BEM

We study theoretically the structural and dynamical properties of metallic nanostructures, free-standing or supported on surfaces. These systems are very interesting from the basic point of view because of the emergence of quantum phenomena, which in turn can be the basis for applications as electronic or optical devices. We are working on two different research fields.

- **Electronic structure, dynamics and spectroscopy of metallic overlayers and nanocontacts.**
We have studied quantum size effects and quantum electronic transport along metallic nanowires or nanocontacts. At the nanometer level electronic current doesn't follow Ohm's law but it is quantized, due to electron confinement. We are motivated by experiments with the MCBJ (Mechanically Controllable Break-Junction) technique developed in the 90s, in which the conductance is measured as nanocontacts are formed and broken.
We are also interested on the lifetime of electrons in metallic islands or films of a few atomic layers grown on surfaces, as Pb on Cu(111). In these systems electrons are confined in the direction perpendicular to the surface, forming the so-called quantum well states (QWS). We calculate the energy and lifetime of electrons, which are fundamental properties that can be probed in photoemission or Scanning Tunneling Spectroscopy (STS) experiments.
Our calculations are based on a variety of complementary theoretical tools which involve many-body and one-electron stationary and time-dependent treatments as Density Functional Theory (DFT) within the local density approximation (LDA), many-body perturbation theory within the GW approximation and wave packet propagation method (WPP)
- **Optical properties and electron transport in plasmonic cavities.**
Another research line is focused on the electromagnetic response of metallic nanostructures when they are excited with external sources as electron beams (electron microscopy) or light (optical spectroscopy). In both cases resonant oscillations of free electrons in the nanostructures, called plasmons, are produced. We are especially interested on the plasmonic properties of metallic nanoparticle dimers. Our goal is to be able to extract information about the electronic transport through molecular linkers connecting two nanoparticles from the changes in the optical extinction spectra in the visible and near infrared frequencies.
In these problems we solve Maxwell equations using dielectric theory and the Boundary Element Method (BEM).

Some of the subjects reported above are part of the thesis defended by Eduardo Ogando in 2004 "Quantum size effects and stability of nanostructures", by Olalla Pérez-González in 2011, "Optical properties and high-frequency electron transport in plasmonic cavities", and by Asier Zugarramurdi in 2012, "Electronic structure, dynamics and spectroscopy of metallic nanosized systems: Pb thin layers and Na nanocontacts".

In all the projects we collaborate with the Department of Materials Physics, DIPC and Unidad de Física de Materiales, Centro Mixto CSIC-UPV in San Sebastian.

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Magnetism and Magnetic Materials group

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Nanomagnetism, Ferromagnetism shape memory alloys, Thin films, Magnetic sensors and actuators

The Magnetism and Magnetic Materials group started working at the Faculty 20 years ago. As a result of the consistent and productive research performed, the group is acknowledged as a consolidated research group. The main objective of the group is to prepare and characterize new magnetic materials with special properties for outstanding applications.

Nowadays the main research lines are the following:

Nanostructured thin films magnetic materials

The study of the magnetic properties of nanomagnets is an issue of enormous interest due to their potential applications as magneto- and bio-electronic devices. The physical properties of nanostructures can be markedly different from those of bulk materials. If the reduction in size reaches a few nanometers, striking phenomena like giant magnetoresistance or magnetic coupling through non-magnetic spacers appears and plays a crucial role in determining the magnetotransport, magnetic moment and magnetic interactions.

Ferromagnetic Shape Memory Alloys (FSMA) in bulk, composite and thin film form

FSMA are active materials that undergo large deformations (up to 10% for some NiMnGa alloys) under the effect of mechanical stress and magnetic field in very short times (a few milliseconds). They present also basic aspects that are attractive for a materials scientist, as the analysis of the magnetic moment (most are typical Heusler alloys) very sensitive to atomic order, multiple structural transitions (premartensitic, martensitic, intermartensitic), large magnetoresistance, etc.

Giant Magneto Impedance (GMI) thin films and devices

The GMI effect produces huge changes in the electric impedance of a soft magnetic material and provides excellent sensitivities to small magnetic fields. It is already used in sensor devices to measure orientation (inside the Earth magnetic field) and other applications. The actual trend is to produce GMI material in the form of thin films to obtain miniaturized devices that can be integrated in microelectronic circuits.

Magnetolectric (ME) phenomena and devices

The ME effect consists on the voltage induced in a material due to its piezoelectric properties when suffering the effect of an applied magnetic field. It is an extremely sensitive effect, and new laminate composites with magnetostrictive elements + high temperature piezopolymers are being developed in our laboratories.

The techniques currently employed by the group include:

- Pulsed Laser Deposition technique (in house technique)
- Sputtering technique (in house technique)
- Atomic/Magnetic Force Microscopy (AFM/MFM) (in house technique)
- Magneto-optical Kerr effect Microscopy (in house technique)
- On-wafer and in-circuit high frequency characterization facilities (in house techniques)
- Photolithography Laboratory (in house technique)
- SQUID magnetometer (SGiker facility)
- Vibrating Sample Magnetometer (SGiker facility)
- Neutron Techniques (Great European Installation Facilities: ILL, ISIS)
- Synchrotron Radiation Techniques (Great European Installation Facilities: ESRF, Diamond)

More information about the group in the web page: www.gmmmt.net

Modelling and implementation of multidimensional electronic systems for Computational Intelligence applications

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KEY WORDS: digital electronics, system modelling, embedded systems, field-programmable gate arrays (FPGAs), computational intelligence, intelligent environments, internet of things (IoT), sensor networks

The main objectives of the “Group of Digital Electronics Design” are: i) basic research, application and synthesis of models for nonlinear dynamic systems, ii) applied research and efficient developments of embedded electronic systems, and iii) study and development of innovative applications in the field of Computational Intelligence (mainly Neural Networks, Genetic Algorithms, and Fuzzy Systems) for all those fields of applied interest (Ambient Intelligence, Robotics and Vision, Biosystems, Intelligent Control, etc.).

RECENT APPLICATIONS DEVELOPED BY THE GROUP

Intelligent environments (IE) should be able to capture and process information from multiple sensors using embedded electronic systems capable of responding in real-time. The complexity and high dimensionality of these electronic environments lead to consider simplifying elements, both in modelling and in their synthesis, with the aim of improving their efficiency and performance. The group has reported the development of a single-chip electronic device, based on reconfigurable hardware, which autonomously acts on IE anticipating user preferences and needs. It is a self-organizing system, without reliance on a central processor, suitable for integration into a network of autonomous cooperative devices. This is a key feature toward the integration of the system into the *Internet of Things*, a new trend in the context of ubiquitous computing and ambient intelligence. Computational Neuroscience is the study of brain function in terms of the information processing properties of the structures that make up the nervous system. It is an interdisciplinary science that links the diverse fields of neuroscience and cognitive science with electrical engineering, computer science, mathematics and physics. A key work in this field is the “HH model” proposed by Alan Lloyd Hodgkin and Andrew Huxley in 1952. This model describes the ionic mechanisms underlying the initiation and propagation of action potentials in the squid giant axon (they received the Nobel Prize for this work in 1963). Although several hardware implementations of the HH model can be found in the literature, our group has developed the first complete digital circuit that emulates this model. The main contribution of this work consists in the use of piecewise linear approximations with variable precision to reduce the computational complexity of the neuron.

Image recognition systems are widely used in different industries such as production plants to detect faulty components on a conveyor or as surveillance systems that are capable of detecting intrusion, differentiating people or observing their motion. What all these systems have in common is the use of high performance cameras and powerful computers with few constraints in power consumption, real-time behaviour, size or cost. In autonomous mobile systems such as mobile manipulators the framework is very different. Object positions and environmental conditions have to be acquired in real-time. Visual servoing is a useful capability for both manipulator arms and mobile robots. However, fast and computation intensive tasks are difficult to implement in small and low power consumption electronic systems required in robot-like systems. The group has developed an electronic object recognition system for an autonomous robot based on a neural network.

Finally, part of the group participates in an industrial project with several companies. The main objective of the project consists in using Computational Intelligence techniques for modelling the behaviour of a co-generation plant with the aim of improving its efficiency.

EOLO group, climate, meteorology and environment

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KEY WORDS: climate, statistical downscaling, atmospheric pollution, mesoscale model.

The EOLO group has made contributions in three main areas of research:

1. Analysis of observed and modelled atmospheric and climatological data
2. Use of advanced statistical techniques for classification and forecasting of different variables at the regional scale (downscaling).
3. Use of mesoscale numerical models (MM5 formerly and WRF currently) for downscaling, hindcast and diagnosis of meteorological events and processes

DATA ANALYSIS

The data-analysis studies have covered diverse areas such as the variability of temperature and precipitation, SO₂ or ozone concentrations, sea surface temperatures and currents and counts of cloud to ground lightning discharges. The relationship of these fields and the large-scale structure of atmospheric fields such as geopotential, wind speed, moisture, moisture transports or convective activity has been examined in detail.

STATISTICAL DOWNSCALING

In this field, the members of the group have prepared methodological advances in deterministic and probabilistic (bayesian) precipitation forecasts, both at the climatological scale and also for precipitation forecasting with very short lead times. Statistical downscaling techniques have been used for practical applications ranging from operational seasonal forecast of temperature, atmospheric pollution or quantitative precipitation forecasts to moisture transports.

MESOSCALE NUMERICAL MODELS

The group has used the MM5 mesoscale model since 2003 and has migrated since 2007 to NCAR's next generation model, WRF. The studies with these models have covered areas such as downscaling in climatological (long) time-scales, testing the behaviour of the different parameterizations that can be used in the model over the Iberian Peninsula. The outputs of long integrations with the mesoscale model have also been used in other practical applications, particularly covering precipitation forecasts. The model has also been used in basic research, such as the study of the atmospheric tides over the Pyrenees.

PROJECT FOR FUTURE WORK

Our aim is to combine the estimations of atmospheric moisture from different sources (in-situ estimations using soundings), several remote sensors such as GPS, satellite and so on and background fields from 3DVAR assimilated fields in order to close the moisture balance for big basins at different time scales, particularly focusing on data-rich periods during the extensive experimental campaigns of the HYMEX project.

Further information on projects and publications can be found at our WEB page: <http://www.ehu.es/eolo>.

Calorimetric, optical and neutron diffraction experiments on the martensitic transformation of Cu-Al-Ni shape memory alloys

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KEY WORDS: martensitic transformations, shape memory alloys.

The specific heat of the martensitic phase transformation shown by Cu-Al-Ni powdered polycrystalline shape memory alloy (SMA), has been measured by adiabatic calorimetry. These results have been compared with the ones obtained for single-crystals of the same alloys, which show the influence of the powder particle size in the martensite plate nucleation and in the well known Temperature Memory Effect (TME) [1]. This is characterized by a neat delay of the transformation to higher temperatures and is explained by the martensitic accommodation process, which makes the elastic energy stored in the plates to be dependent on the thermal history [2, 3]. A simple thermodynamic approach, which accounts for this effect and for the martensitic transformation, has been developed. In addition, optical microscopy has been used to confirm these phenomena on qualitative grounds. Finally, neutron diffraction experiments have been performed around the transformation temperature range to obtain information about the microscopic mechanisms underlying the observed thermodynamic behaviour.

[1] G. Airoldi, A. Corsi and G. Riva. *Scripta Materialia* 36, 11 (1997) 1273

[2] J. Rodríguez-Aseguinolaza, I. Ruiz-Larrea, M. L. Nó, A. López-Echarri, and J. San Juan. *Journal of Applied Physics* 107 (2010) 083518.

[3] J. Rodríguez-Aseguinolaza, I. Ruiz-Larrea, M. L. Nó, A. López-Echarri, and J. San Juan. *Intermetallics* 18 (2010) 2183-2190.

Crystallography online by the Bilbao Crystallographic Server

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KEY WORDS: Crystallographic Symmetry, Phase Transitions, Online Tools.

The *Bilbao Crystallographic Server* (<http://www.cryst.ehu.es>) website offers crystallographic databases and programs. It can be used free of charge from any computer with a web browser via Internet. The server has been operating for more than ten years, and new programs and applications are constantly being developed. The aim of the present contribution is to report on the current state of the server and to provide a brief description of the accessible databases and programs.

The server is built on a core of databases and contains different shells. The set of databases includes data from *International Tables of Crystallography*, Vol. A: *Space-group symmetry*, and the data of maximal subgroups of space groups as listed in *International Tables for Crystallography*, Vol. A1: *Symmetry relations between space groups*. There is an access to the crystallographic data for the subperiodic layer and rod groups. A k -vector database with Brillouin zone figures and classification tables of the k -vectors for space groups is also available. Very recently, the Magnetic Space Groups data with general positions and Wyckoff positions for different settings, along with systematic extinction rules have also been incorporated into the server and a new shell has been dedicated to the related tools (MGENPOS, MWYCKPOS, MAGNEXT).

The third shell contains applications which are essential for problems involving group-subgroup relations between space groups. Given the space group types of G and H and their index, the program SUBGROUPGRAPH provides graphs of maximal subgroups for a group-subgroup pair $G > H$, all the different subgroups H and their distribution into conjugacy classes. The Wyckoff position splitting rules for a group-subgroup pair are calculated by the program WYCKSPLIT.

The next shell includes programs on representation theory of space and point groups. REPRESENT constructs little group and full group irreducible representations for a given space group and a k -vector, CORREL deals with the correlations between the irreducible representations of group-subgroup related space groups. The program POINT lists character tables of crystallographic point groups, Kronecker multiplication tables of their irreducible representations and further useful symmetry information.

Parallel to the crystallographic software, we develop a shell with programs facilitating the study of specific problems related to solid state physics and structural chemistry. The program PSEUDO performs an evaluation of the pseudosymmetry of a given structure with respect to supergroups of its space group. AMPLIMODES performs the symmetry-mode analysis of any distorted structure of displacive type. The analysis consists in decomposing the symmetry-breaking distortion present in the distorted structure into contributions from different symmetry-adapted modes. Given the high and low symmetry structures, the program calculates the amplitudes and polarization vectors of the distortion modes of different symmetry frozen in the structure. The program SAM calculates symmetry-adapted modes for the centre of the Brillouin zone and classifies them according to their infrared and Raman activity. NEUTRON computes the phonon extinction rules in inelastic neutron scattering. Its results are also relevant for diffuse-scattering experiments.

A set of structure utilities has been included for various applications such as: the transformation of unit cells or complete structures; strain tensor calculation, assignment of Wyckoff Positions; equivalent descriptions of a given structure; comparison of different structures with the recently added support for the affine normalizers of monoclinic space groups. A new tool, STRUCTURE RELATIONS calculates the possible transformation matrices for a given pair of group-subgroup related structures. Summarizing, the tools located on the server can be combined to analyze, calculate and visualize problems of structural and mathematical crystallography, providing a collection of applications under the same working environment.

Novel properties of materials under extreme conditions

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KEY WORDS: quantum mechanics, ab-initio calculations, high pressure, electronic excitations

Simulating and understanding the many different physical properties of solids is a great challenge. From superconductors to the recently discovered topological insulators, quantum mechanics reveals striking properties of materials under extreme conditions. What is, for instance, the reason of the anomalous magnetic field measured in Jupiter, or the unexpected brightness of Uranus?

The answer may well be associated to the complex electronic properties induced by the high pressure conditions of the inner core of these two dense planets. Without the need of traveling so far, the combination of modern theoretical techniques and powerful computational resources provides the necessary tools for analyzing and understanding the properties of materials under such extreme conditions.

Our research is devoted to first-principles theoretical investigations of many physical phenomena related to electronic excitations, dynamical response. In particular, we are working on the following topics:

1. Materials under pressure

High pressure research poses strong theoretical challenges on the prediction of novel phases of materials. Under pressure, core electrons overlap leading to an electronic complexity not expected at ambient conditions. Notable examples of the properties arising from these extreme conditions are the superconducting in lots of compounds as we have demonstrated in the group IV hydrides that may reach at T_c of 60K at high pressure. What is more, we have thoroughly studied the high pressure superconducting phases of calcium, which is the element that reaches the highest T_c.

2. Spintronics

Since the rather unexpected discovery of spin-split Shockley-type surface states on the Au [111] surface, the theory of the spin polarization on two dimensional systems has attracted an increasing scientific interest during the last decade. Mostly due to the potential of the emerging field of spintronics and the very recently discovered topological insulators, the efforts to understand the relativistic electronic structure of the surface electrons has acquired a great importance. In this context, we develop a method for analyzing spin-flip excitations upon the spin-polarized surface states utilizing Wannier function interpolation.

Shape Memory Alloys at Micro and Nano - scale

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KEY WORDS: shape memory alloys, martensitic transformations, electron microscopy, nano-indentation

The research group on Physical Metallurgy and Phase Transformations is considered as a Consolidated Research Group A from the Basque Government, with three main research lines:

- * Shape Memory Alloys (SMA): Shape memory alloys are considered as smart materials because of the shape memory and superelastic properties, which allows its use as sensor and actuators in many industrial sectors. We elaborate polycrystals and singlecrystals of several Cu-based SMA for intermediate temperature applications (-100°C to 200°C), in particular Cu-Al-Ni and Cu-Al-Be. A complete microstructural and thermomechanical characterization is being performed in the developed alloys, in order to optimize the microstructure to exhibit performant thermomechanical properties for practical applications [1-5].
- * High Temperature Intermetallics: Intermetallic Aluminides are being developed as the new material's generation to be used in engines for aeronautic. Our interest is focused on the mobility of defects which control the deformation of these materials at high temperature, but the approach is through the study of the relaxation processes, having place in the temperature range of interest, by mechanical spectroscopy complemented by electron microscopy. At present we are working on Fe-Al and Ti-Al alloys [6,7].
- * SMA for MEMS: Shape memory alloys offer the highest work-output in comparison with other functional materials, and are seriously considered to work as sensors and actuators in Micro Electro-Mechanical Systems (MEMS). We approached an ambitious study on the behaviour of SMA at micro and nano scale, and we showed that Cu-Al-Ni exhibit excellent properties at micro-nano scale. We are pioneers in this field and discovered a size-effect on the superelastic behaviour [8-10]. This is the selected topic for the Poster.

- [1] M.L. Nó, D. Caillard, J. San Juan. A TEM study of martensitic habit planes and orientation relationships in Cu-Al-Ni shape memory alloys. *Acta Materialia* 57 (2009) 1004-1014.
- [2] J. Rodríguez-Aseguinolaza, I. Ruiz-Larrea, M. L. Nó, A. López-Echarri, and J. San Juan. Temperature memory effect in Cu-Al-Ni shape memory alloys studied by adiabatic calorimetry. *Acta Materialia* 56 (2008) 3711-3722.
- [3] M. Barrado, G.A. López, M.L. Nó, J. San Juan. Composites with ultra-high damping capacity based on powder metallurgy shape memory alloys. *Materials Science and Engineering A* 521 (2009) 363-367.
- [4] M.L. Nó, A. Ibarra, D. Caillard, J. San Juan. Quantitative analysis of stress-induced martensites by in-situ transmission electron microscopy superelastic tests *Acta Materialia* 58 (2010) 6181-6193.
- [5] I. López-Ferreño, T. Breczewski, I. Ruiz-Larrea, A. López-Echarri, M.L. Nó, J. San Juan. Thermal treatments and transformation behavior of Cu-Al-Be SMA. *Journal of Alloys and Compounds* (2012) in press.
- [6] P. Simas, J. San Juan, M.L. Nó. High temperature relaxation analysis in a fine-grain B2 Fe-Al intermetallic. *Intermetallics* 18 (2010) 1348-1352.
- [7] P. Simas, T. Schmoelzer, M.L. Nó, H. Clemens, J. San Juan. Mechanical Spectroscopy in Advanced Ti-Al-Nb-Mo Alloys at high temperature. *Mater. Res. Soc. Symp. Proc.* 1295 (2011) 139-144.
- [8] J. San Juan, M.L. Nó, C.A. Schuh. Superelasticity and Shape memory in Micro and Nanometer-scale Pillars. *Advanced Materials* 20 (2008) 272-278.
- [9] J. San Juan, M.L. Nó, C.A. Schuh. Nanoscale shape-memory alloys for ultrahigh mechanical damping. *Nature Nanotechnology* 4 (2009) 415-419.
- [10] J. San Juan, M.L. Nó, C.A. Schuh. Thermomechanical behavior at the nanoscale and size effects in shape memory alloys. *Journal of Materials Research* 26 (2011) 2461-2469. (Invited Feature Paper).

Infrared radiometry

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KEY WORDS: Infrared radiation, Emissivity, FTIR, Oxidation.

It is a recently created research group (July 2002) in infrared radiometric studies and measurements. During the first years, a radiometer for direct infrared spectral directional emissivity measurements was designed, constructed and calibrated. The device, which is now fully operative, allows the measurement of the spectral emissivity of opaque samples between 1.28 μm and 25 μm , as a function of the temperature between 200 °C and 800 °C, and for emission angles between 0° and 80°. Furthermore, the emissivity can be obtained as a function of the environmental conditions: vacuum or controlled atmosphere.¹

The value of the emissivity is needed for several technological and scientific applications: radiometric temperature measurement (pyrometry), optical constant determination, low observability, high heating efficiency, thermal isolation, solar cells, etc. Additionally, depending on the specific application, low or high emissivity can be required, although, in most of the cases, a selective emissivity is desirable.

According to the possibilities of the experimental device, the following research lines are currently in progress:

- 1- Study and analysis of the measurement method with the goal of improving the radiometer performance.
- 2- Study and control of the emissivity of aeronautic alloys used in aircraft turbine engines. This project is carried out in collaboration with Industria de Turbopropulsores, S.A.
- 3- Study and characterization of the emissivity of cutting tools and some test materials used in the machining industry, so as to model and optimize the machining process. This work is done in collaboration with the Mondragon Unibertsitatea.
- 4- Application of infrared emissivity measurements to the study of in situ oxidation processes at high temperature (till 850°C). These studies lead to information about the oxidation mechanisms and the activation energy.

In the near future, it is planned to open new research areas: Optical constant determination in thin films, emissivity measurement at ambient temperatures by using both direct and indirect methods, etc.

Finally, it is important to remark that the radiometer developed in the laboratory is the only one in Spain, although there are similar and complementary ones in international reference laboratories. This permits to offer a unique service of reliable absolute emissivity measurements to other laboratories and enterprises.

Physical and mathematical fundamentals of Universe structure

J.M Aguirregabiria Aguirre, T. Broadhurst, A. Chamorro Belmonte, C. Escamilla Rivera, A. Feinstein, I. Garay Elizondo, J. Ibáñez Medrano, R. Lazkoz Sáez, J. Lizarraga Olano, J.M Martín Senovilla, B. Reina Valdemoros, M. Rivas Pérez, V. Salzano, I. Sendra Server, J. Urrestilla and R. Vera Jiménez

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KEY WORDS: gravitation, general relativity and cosmology.

Einstein Equations (or modifications) represent a balance between the geometrical properties of spacetime and the physics of non-gravitational fields, being the fundamental framework for the study of the Universe. Moreover, for a complete comprehension it is necessary a deeper study of its first stages, dominated by high energy processes, and the physical laws that govern them. Thus, Cosmology is tightly related to other aspects of the Universe structure and to the underlying mathematical nature.

Theoretical and Phenomenological Cosmology

J.M Aguirregabiria Aguirre, T. Broadhurst, A. Chamorro Belmonte, C. Escamilla Rivera, A. Feinstein, I. Garay Elizondo, J. Ibáñez Medrano, R. Lazkoz Sáez, J. Lizarraga Olano, J.M Martín Senovilla, B. Reina Valdemoros, M. Rivas Pérez, V. Salzano, I. Sendra Server, J. Urrestilla and R. Vera Jiménez
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KEY WORDS: gravitation, general relativity and cosmology

This line of work involves different theoretical and phenomenological aspects of the Universe within the framework of the General Relativity and a wider context of modified theories. This area of research given the forthcoming large number and quality of observational data. Roughly speaking this data will give us the chance of obtaining conclusions about the possible components of the Universe whose presence can be inferred through the kinematics of the Cosmos at different scales. One of the aspects that generates a major challenge is the apparent acceleration of the expansion of the Universe.

Magneto-electric Multi-ferroics: functional materials with double perovskite layered structure

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KEY WORDS: multi-ferroics, double perovskites, layered ordering.

Understanding of the interrelationship between structure, thermodynamic properties and phase diagrams is very useful for rationalizing the behavior of materials and development of predictive models, which can be used to optimize the composition of materials and their fabrication processes. The properties of materials are governed by its electronic and crystallographic structure. Chemical bonding determines the electronic structure of materials. Furthermore, the electronic structure plays a predominant role in determining the physical, electrical, magnetic, thermal and optical properties of materials. Crystal structure also influences most properties of materials. Since changes in thermodynamic variables such as temperature, pressure, and composition dramatically alter the physical properties of materials and its structure, it is desirable to study the thermodynamic stability of materials in conjunction with phase relations. Phase diagrams can indicate the ranges of pressure, temperature and chemical composition where specific phases and mixtures of phases are stable. To materials scientists phase diagrams are like maps to travelers. They guide the path through the composition space to find phases, fulfilling specific materials performance requirements.

Focus of the present investigation is to obtain correct phase relations and accurate thermodynamic data in selected technologically important ceramic oxide systems in which the data are either not available or are inconsistent.

Typical multi-ferroic magneto-electric (MM) materials pertain to the group of perovskite transition metals oxides and include rare-earth manganite and ferrites; some others are bismuth compounds, for instance. In those compounds ferroelectricity is either an independent phenomenon or it is an induced effect of the magnetic ordering. Some new materials have been proposed to show MM properties: materials with the general formula $AA'BB'O_6$, but in which a layer ordering scheme of the A and A' site cations gives rise to a different set of possible structural symmetries.

With this kind of ordering it can be demonstrated that the highest possible symmetry is described by the space group $P4/nmm$ (#129), and one of the subgroups of that space group is $P21$ (#4), which is polar. This fact means that in the materials with the mentioned kind of ordering the ferroelectricity is allowed theoretically, and experimentally, if that space group could be found to exist. The presence in the structure of a magnetic cation will give rise to magnetic properties, that eventually can couple to the electric ones, giving rise to the MM properties.

Following some the work done by some research groups on this kind of A-site arrangement and with our experience of the last years working on double perovskites and with materials with related atomic arrangements, we have synthesised some new materials with the mentioned A-site layer arrangement. At present, we have the following materials: $NaLnMWO_6$ ($Ln=La,Nd,Dy$) and ($M=Co,Ni,Mn$) and $NaLaMTeO_6$ ($M=Co,Ni,Mn,Mg$). Despite the fact that many works have been published on this arrangement in the last years for different cations in the B- and B'-sites and in the A- and A'-sites, none has been devoted to the temperature-induced structural phase-transitions. This is the aim of our effort: analyze symmetries, structural and magnetic phases and structural and magnetic phase transitions with the aid of the formalism of the symmetry adapted modes and the proper computer tools.



Kimika/Química

Towards an integrative assessment on global issues in environmental chemistry and cultural heritage

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KEY WORDS: Analytical development; Environmental chemistry; Material analysis

Quite often we face with the effects of chemicals on the living organisms and on materials. In the first case, we deal with the fate and behaviour of contaminants in the environment and, in particular, with the risks associated with the presence of those contaminants for the environmental and the human health. In the second case, we mean the effects on the building materials, artworks or archaeological materials.

Most of those global issues require an integrative approach to understand the processes that take part in the hazardous effects or in the degradation or restoration processes. The role of our work is to study them in order to provide the tools to assess those processes.

IBeA (*Ikerketa eta Berrikuntza Analitikoa*) is a consolidated group with 13 permanent staff members and more than 5 postdocs and 15 PhD students. IBeA leads several research topics in both the environmental chemistry and the cultural heritage and works with many other groups of the UPV/EHU, and from other Spanish and European universities. Together with two other research groups of the UPV/EHU (hydrogeologists and archaeologist), we are active members of the recently nominated UFI Global Change & Heritage.

In environmental chemistry, the most active lines deal with the development of new sampling and analysis methods of micro-contaminants. Their main aims are to study the mechanisms of transport and transfer among the different natural compartments and to support the environmental risk assessment studies. In this sense, we are currently working on (i) the development of analytical methods for emerging pollutants (personal care products and pharmaceuticals) through chromatographic techniques (GC-MS, LC-MS-MS), (ii) the use of passive sampling devices to provide integrative levels of the presence of many contaminants in aquatic and atmospheric media, (iii) on the plant bioavailability processes of some emerging pollutants that can be amended through contaminated sewage sludge that is used as fertilizers and the effect of that bioavailability on human consumption, and finally, (iv) we are also studying the environmental impact of abandoned mines and quarries as well as the assessment of the environmental risks of the reuse of black slags.

In the cultural heritage field, one of the consolidated lines deals with the development of methods and strategies based on the use of non-destructive, non-invasive and hand-held portable equipments, especially when artworks are very valuable objects or they cannot be damaged nor sampled. Techniques such as Raman and infrared (FTIR) spectroscopies, X-ray fluorescence (XRF) or laser induced breakdown spectroscopy (LIBS) are of common use for those purposes. In addition to this, we also use microscopic techniques such as scanning electron microscopy (SEM) or atomic force microscopy (AFM) coupled to elemental and molecular analysis not only to characterise the original components of the objects, but also to determine the degradation products that are formed due to the impact of chemical contaminants or aggressive environmental conditions.

Finally, owing to the use of a wide range of analytical instrumentation and methodologies we have gained the expertise to open new horizons in other fields such as the food analysis and processes (aroma analysis and functional foods), the application of nanoparticle induced surface enhance Raman spectroscopy (SERS) on tissue imaging, or sea/estuarine water acidification processes (accumulation of CO₂).

Natural products in foods, beverages and plants

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KEY WORDS: Polyphenols, anthocyanins, tannins, red wine, fruits juices, agroindustrial residues, plants, antioxidant assays, volatile profile, aromas

Determination of the chemical composition of foods, plants and beverages has a huge interest from many points of view. A deep knowledge of natural products in foods can lead to improve nutritional quality or to detect geographical origins, manufacturing methods, bad practices, or adulterations.

Polyphenols are a very important group of natural products due to their ubiquity in the vegetable kingdom and their interest as a key to explaining many food properties such as flavor, astringency, aroma, and color, besides their many beneficial effects on human health as a lower risk of heart diseases and cancer.

With this aim and after successful works in ciders, apples, txakoli and edible oils, our research group is currently working in the following projects:

- Volatile compounds analysis in txakoli by *multidimensional* gas chromatography coupled with mass spectrometry which are responsible for wine aroma. This feature is critical for the final quality of wine and its knowledge informs the wineries about the course of vinification.
- Development of a fast method for the determination of anthocyanins by using infrared spectroscopy, which is a fast, cheap and widely employed technique in wineries: For this purpose, chemometric tools (PCA, PLS) are employed to correlate infrared spectrum with anthocyanin contents, previously quantified by HPLC-DAD.
- Study of the polyphenolic profile of fruit derived foods, determined by HPLC-DAD and HPLC-MS/MS: This allows detecting adulterations and bad practices in the food manufacturing by using chemometrics (PCA, MLR, PLS, LDA).
- Study of the formation and evolution of anthocyanic derived pigments in different stages of the red wine from "Rioja Alavesa" which are formed in specific reactions during the ageing. These have an impressive variety and structure complexity, whereas their concentrations and relations are fundamental for color and other organoleptic wine properties, as well as for the final type of wine. Fractions are analyzed by HPLC-DAD-MS/MS.
- Study of Tannins in aged red wines from Rioja, which define to a great extent many properties of wine, like astringency and wine texture: Study of this group of polyphenols results in a hard task due to the great diversity of their structures and polymerizations and their matrix complexity. Therefore, complicated multi-step separation procedures must be developed by making use of solid-phase extraction (SPE), liquid-liquid extraction (LLE) and selective evaporation of the solvent, SEC, and HPLC.
- Study of the polyphenolic profile of different plants with medicinal use. Determined by HPLC-DAD and HPLC-MS/MS. The great diversity of compounds that are present in plants can be a big source of natural remedies.
- Characterization of apple pomace, a by-product of apple cider processing industry with a high polyphenolic content and antioxidant activity. An HPLC-DAD method has been developed to the identification and quantification of polyphenols. Besides, two assays of antioxidant capacity (ABTS⁺ and DPPH'), an assay to determinate the total polyphenols and another one for total flavan-3-ols have been carried out.

FARMARTEM

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KEY WORDS: drugs analysis, metabolomics, pesticides, microencapsulation, fluorinated compounds, documents

FARMARTEM is an analytical chemistry research group involved into different fields: determination of drugs and metabolomic studies, environmental and industrial analysis, and forensic studies of documents.

DETERMINATION OF DRUGS AND METABOLOMICS

The drug analysis in biological fluids is the more consolidated research line of this group. Determination of drugs used in combined cardiovascular therapy in biological fluids (plasma, urine, saliva) have been carried out using selective and sensitive analytical techniques: high performance liquid chromatography-mass spectrometry (HPLC-MS) and ultra high performance liquid chromatography-mass spectrometry (UHPLC-MS). Different sample treatments (protein precipitation, solid phase extraction, -pippette-tip extraction and solid phase microextraction) have been used due to the complexity of matrixes, analytes low concentrations and reduced volume of sample.

Nowadays an analytical method for the determination of the muscle-relaxant rocuronium concentration in muscle tissue microdialyzates is being developed. This method will allow the study of the pharmacokinetic and pharmacodynamic of this drug in order to design an automated dosage model. On the other hand metabolomics is the latest line introduced in the group and is focus to the search of maturity biomarkers in children and the study of the metabolic pathways altered by squizophrenia disease. In both cases the analytical technique utilized has been liquid chromatography coupled with mass spectrometry.

ENVIRONMENTAL AND INDUSTRIAL ANALYSIS

In this research line, different multidisciplinary projects have been done. Analytical methods for the quantification of pesticides in several environmental matrixes have been developed and applied to water analysis and soils bioremediation studies. The microencapsulation of biocides is other innovative area in which the group is involved. The advantages of microencapsulated biocides for the environment have been demonstrated. The use of natural products obtained from plants in the production of a specific and with great efficacy biocide for the plagues control is other objective of this environmental line in collaboration with chemical companies.

Moreover, analytical methods for quality control analysis of inorganic fluorinated compounds (cationic and anionic impurities) by ion chromatography and capillary electrophoresis are being developed.

FORENSIC STUDIES OF DOCUMENTS

In this research line, three different topics can be distinguished:

- Optic analysis of inks: They allow to detect documental manipulations and to identify writing tools (ballpoint pens, felt-tip pens, markers...).
- Characterization and dating of inks: It is possible to determine the age of a document by liquid chromatography-mass spectrometry and/or gas chromatography-mass spectrometry.
- Analysis of toners and printed inks: These analyses are very useful to differentiate toners of laser printers from toners of photocopiers, and inks of liquid inklet printers from hand writing inks.

Nanometric Hybrid Materials with Optoelectronic, Catalytic and Mechanical Properties.

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KEY WORDS: Laser Dyes, Zeolite, AlPO, layered Clays, Metal Organic Framework, Micropores, Atomistic Simulation.

Actually, the encapsulation of organic fluorophores into nanostructured hosts is an active area of research. This kind of hybrid materials opens the door to a wide variety of photoactive devices with promising application in many technological and commercial fields. The solid framework offers a rigid and robust environment for fluorescent molecules improving the emission capacity and thermal stability and infers a high organization degree. In this sense, the photophysical characterization of the dyes and dye-doped materials is a key factor to understand the involved processes or to develop new dyes with tailor-made physicochemical properties. Accordingly, quantum mechanical simulations have become a powerful tool to complement the experimental work and orient future strategies.

The Molecular Spectroscopy Group has accumulated a vast experience in the photophysical characterization of fluorophores (coumarines, rhodamines, BODIPY, pyronine, styryls, oxazines) with emission ranging from ultraviolet to the red part of the visible. To perform such study the laboratory is equipped with spectroscopic (absorption, and steady-state and time-correlated fluorescence) and microscope (confocal fluorescence) techniques. These dyes have been characterized not only in solution but also in polymers, clays, zeolites and aluminophosphates as dopants. The obtained materials are being successfully applied in dye lasers, sensors and antenna devices, as result as the consolidated collaborations established by the group in the last years.

Among the different research tasks of the group, four main research lines should be highlighted:

1. **BODIPY dyes** are being exhaustively study by the scientific community as is revealed by the vast number of publications dealing about them. One of mayor advantage of BODIPYs is that their molecular structure can be modified almost in the desired way. Thus, the photophysical properties can be controlled by the substitution pattern. Our interest in this field is focused on the spanning of their fluorescence and lasing region to the blue as well as to the red part of the visible. Furthermore, their chemical stability allows their use as sensors to monitor the environment characteristics or detect the presence of an analyte.
2. The encapsulation of guest **fluorophores into the unidimensional pores of zeolite L and AlPO-5 and into a well-organized 2D-multilayer of clay films** leads to photoactive materials with interesting properties form applications such as antenna and white-light emitting devices, non-linear optics, catalysis or photovoltaic cells. These nanomaterials are characterized by a high organization degree where the molecule is aligned in a preferred position due to the geometrical restrictions imposed by the solid framework.
3. **Porous coordination polymers (PCPs) or metal-organic framework (MOFs)** are considered as a functional class of porous materials. The designability by varying the nature of the coordination metals and the organic linkers, the cristallinity in their structures resulting in nanometer-size confined spaces and the flexibility by the entanglement of their frameworks are unique properties for the development of multiple applications such as gas storage and separation, heterogeneous catalysts and molecular sensors. The design of a PCP with photoactive entities as part of the structure and whose luminescent properties are highly sensitive to guests can offer potential application as luminescent sensor
4. The properties of **molecules confined in micropores** are far distant from those in solution. The confinement and close interaction with the substrate affects their mobility, orientation, and electronic properties. Furthermore, they might induce changes in the substrate. Atomistic simulation is a versatile tool to understand the effect on confinement on the guest molecules and the host structure, relevant for the design of a wide range of materials, from hybrid solar cells to fracture resistant cement.

Smart materials

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KEY WORDS: Nanoparticles, shape memory, smart polymers, sensors and actuators

Smart materials or multifunctional materials are materials having one or more properties (shape, viscosity, color,...) that can be significantly changed in a controlled fashion by external stimuli, such as stress, temperature, moisture, pH, electric or magnetic fields.

Since smart materials first started to play an important role due to their capabilities to respond actively to environmental stimuli and enable significant potential applications, research on such materials has been progressively growing. The potential applications of such smart materials are abundant, and include the design of smart aircraft skin embedded with fiber optic sensors to detect structural flaws; bridges with both sensor and actuating elements to counter violent vibrations; flying microelectromechanical systems (MEMS) with remote control for surveying and rescue missions; and stealth submarine vehicles with swimming muscles made of special polymers.

Our laboratory focused on the design and the synthesis of smart materials with susceptible properties to be useful as sensors and/or actuators. In this topic we are working in different research lines with the aim to develop new materials of different nature (organic, inorganic and hybrid) with specific properties as, for example, piezoelectric, shape memory and conducting polymers.

RESEARCH LINES

- **Shape memory polymers.** A series of thermally induced shape memory polymeric systems from commercially available semicrystalline polyalkenamer are obtained by a controlled crosslinking mechanism via free radical reactions. Moreover, functional composites with enhanced mechanical performance, polymer blends able to perform several subsequent shape changes, and polymeric systems with remote activation of shape memory effect are being developed and evaluated too.
- **Piezoelectric polymers.** The development of polymers with piezoelectric properties at high temperature is being studied. For this purpose, polyimides have been chosen due to their excellent thermal, mechanical and dielectric properties. Piezoelectric polyimides with orientated polar groups into the polymer backbone are obtained.
- **Intrinsically conducting polymers.** Synthesis and development of intrinsically conductive polymers through chemical modifications in the polymer backbone in order to improve their conductivity properties depending on the specific application.
- **Smart polymer surfaces.** Synthesis of smart polymer surfaces through the formation of inter-polymer complexes whose formation and disruption may be controlled by the environmental conditions (temperature, pH,...).
- **Synthesis of nanoparticles.** Synthesis, characterization and modification of magnetic nanoparticles for biological applications; polymer coated iron nanoparticles have been synthesized by the microemulsion method which affords great control over the size and shape of the nanoparticles.

Determinations of Local Spins in the Physical Space

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KEY WORDS: local spins, reduced density matrices, spin density.

During the last decade there has been a considerable interest in studying procedures to decompose the expectation value of the spin-squared operator $\langle S^2 \rangle$ corresponding to an N-electron system into one- and two-center components. These quantities (local spins) provide the determination of the spin state of an atom or group of atoms in a molecule, as well as the description of magnetic interactions between the atoms which compose the system. This information becomes particularly interesting in the study of complexes of transition metal which play an important role in various disciplines as catalysis, enzyme chemistry, etc.

Clark and Davidson have proposed a procedure to decompose the $\langle S^2 \rangle$ quantity that utilizes projection operators associated with atomic centers or larger fragments within a molecule [1]. Alternatively, the direct partitioning of the expectation value $\langle S^2 \rangle$ has also been reported [2]. We have described the partitioning of the expectation value of $\langle S^2 \rangle$ in terms of the spin-density matrix elements and those of the cumulant matrix of the second-order reduced density matrix [3-6]; the results, obtained in the Hilbert space of atomic orbitals have been discussed in detail. The main aim of this work is to complement this kind of studies describing our treatment in the three-dimensional physical space, using the domains associated with the Bader atoms-in-molecules theory and the technique of fuzzy atoms [7]. The results show the reliability of the three-dimensional partitioning for detecting local spins, in good agreement with the genuine chemical knowledge, and reveal a slight lower basis-set dependence compared with those arising from the Hilbert space.

[1] A.E. Clark, E.R. Davidson, J. Chem. Phys. 115, 7382 (2001)

[2] I. Mayer, Chem. Phys. Lett. 440, 357 (2007)

[3] D.R. Alcoba, L. Lain, A. Torre, R.C. Bochicchio, Chem. Phys. Lett. 470, 136 (2009)

[4] A. Torre, D.R. Alcoba, L. Lain, R.C. Bochicchio, J. Phys. Chem. A 114, 2344 (2010)

[5] L. Lain, A. Torre, D.R. Alcoba, R.C. Bochicchio, Theor. Chem. Acc. 128, 405 (2011)

[6] D.R. Alcoba, A. Torre, L. Lain, R.C. Bochicchio, J. Chem. Theory Comput. 7, 3560 (2011)

[7] D.R. Alcoba, A. Torre, L. Lain, R.C. Bochicchio, Chem. Phys. Lett. 504, 236 (2011)

Size Matters: *Smart Nanocarriers for Biomedical Applications*

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KEY WORDS: Cancer, nanogel, swelling, drug release

In the last decade, nanoscience has taken a growing interest because of the wide range of potential applications that can bring in areas such as biomedicine (drug release), agriculture, the cosmetics industry, polymer science, etc. Undoubtedly, the complexity of nanotechnology involves the use of new techniques for structuring and chemical functionalization exploiting the most of the properties of nanoparticles to enable its use on a selective or specific manner.

The so-called stimulus-response smart nanogels have emerged as a promising new class of materials with pharmaceutical applications. In these systems, small changes in some environmental variable such as temperature, pH, ionic strength, leads to a reversible phase transition in the structure of the gel. Furthermore, when these materials have ionizing functional groups are sensitive to changes in pH. The pH affects these systems similarly to temperature, so that a given change in pH of the medium makes the nanogel to swell, leading to an increased pore size of the polymer network, this facilitate molecules migration toward outside of the nanogel. This process is known as "release" and is the principle governing the current drug dispensing systems. Within the drug dosing systems we can find two basic types, which are the starting point for designing new mechanisms of transport and drug delivery, these are called "controlled release" and "targeted release".

One of the most promising strategies in anticancer therapies is the targeted delivery through malignancy-associated cellular markers. Recently, Katime and coworkers have designed new synthetic devices with enhanced stimuli-responsive sensitivity and targeting ligands that can be a promising field for the development of cancer-specific delivery systems. The new devices would lead to a reduction in the minimum effective dose of the drug required for each target. The over-expression of folate receptors on many cancers identifies them as a potential target for a variety of ligand receptor-based cancer therapeutics. In fact, folate receptors are qualified as a tumor-specific target. Furthermore, folic acid molecules have numerous advantages in comparison with other ligands, such as their small size, availability, simple chemical conjugation, and no immunogenicity. Due to these unique characteristics folic acid is actually presented as an ideal ligand for targeted delivery into tumors. Katime et al. have developed new synthetic molecules based on microemulsions systems that can offer an interesting and potentially quite powerful alternative carrier system for drug delivery because of their high solubilization capacity, transparency, thermodynamic stability, ease of preparation, and high diffusion and absorption rates when compared to solvent without the surfactant system.

Polyoxometalates. Inorganic Building Blocks for Functional Materials.

Elhuyar's dream alive and kicking

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KEY WORDS: Polyoxometalates, Hybrid materials, Smart surfaces.

Polyoxometalates (POMs) are a large family of anionic clusters composed of oxo-bridged early transition metals from groups 5 and 6. These species are well-known because of their remarkable electronic versatility and structural diversity, which endow them with applications in numerous key areas including catalysis, biomedicine or nanotechnology. Since POMs offer a wide variety of compositions and shapes, they have been regarded as important building blocks for the construction of hybrid organic-inorganic materials, which are subject of great interest due to the possibility of combining active inorganic and organic components in a single material to get unusual structures and/or properties. Thus, a plethora of hybrid compounds made of POMs have been described in recent years

Four research lines within the POM-based organic-inorganic hybrid materials field are currently being developed in our group:

SELF-ASSEMBLED POMs WITH 3d/4f METALS

This line is focused in the synthesis and structural characterization of novel POM clusters with unprecedented structures from the self-assembly of different POM precursors with first-row transition metals and/or rare earths. We are particularly interested in POMs with exposed 3d or 4f metal centers displaying at least two available coordination sites because these POMs could be subject of direct organic functionalization.

POROUS POMOFs

The aim in this line is to synthesize and characterize hybrid metalorganic frameworks from the combination of POMs and first-row transition metal complexes with different organic ligands (POMOFs). These complexes can act as linkers of POMs to construct multidimensional hybrid lattices showing accessible pores or channels, making them good candidates for gas storage or as sensors.

POM-BOX

Bisoxazoline (BOX) complexes are known as suitable enantioselective catalysts for different organic reactions. Since several POMs also display good catalytic activity, our goal is to support BOX complexes in POM surfaces to generate new hybrid molecular species or extended lattices with potential catalytic properties derived from synergistic effects between both components that could improve those from the components alone.

SMART SURFACES

We are also interested in endowing surfaces made of organic polymers with additional properties provided by POMs through covalent anchorage of the latter components to the former surfaces. For this purpose, we have selected polystyrene surfaces with terminal polyacrylic functionalities and POMs with exposed 4f metal centers, in such a way that anchorage is made via coordination of the highly oxophilic 4f centers to carboxylate groups.

New approaches for the development of porous materials based on metal-biomolecule frameworks (MBioFs)

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KEY WORDS: Porous materials, Coordination polymers, Metal-organic frameworks (MOFs), Metal-biorganic frameworks (MBioFs), Supramolecular Metal-biorganic frameworks (*supra*MBioFs) catalysis, gas adsorption and separation.

Metal-organic frameworks (MOFs) are a class of hybrid materials comprising metal ion-based vertices and organic ligands (linkers) that serve to connect the vertices into two or three-dimensional periodic structures. The structures and properties of MOFs can be carefully tailored by judicious selection of metal ion and organic linker building blocks.

A hallmark property of MOFs is their intrinsic porosity, which renders them potentially useful for gas storage, separations, catalysis, and a variety of additional applications that rely on highly specific host-guest interactions. Their promising properties coupled with the ease by which their structures can be modified make MOFs one of the most exciting, diverse, and rapidly growing areas of modern chemistry research.

Many potential applications of MOFs may require them to be constructed from benign building blocks that are biologically and environmentally compatible. For example, most biological applications, including drug delivery or intracellular imaging, would clearly require non-toxic MOF materials. In addition, many proposed applications will require bulk quantities of MOFs. To reduce their environmental impact, bulk MOF materials should be either environmentally compatible or easily recyclable. New generations of MOFs should be designed according to specific composition criteria that address their environmental and biological compatibility.

Recently, biomolecules have emerged as building blocks for constructing Metal-Biomolecule Frameworks (MBioFs). MBioFs are defined as MOFs constructed from at least one biomolecule which serves as an organic linker. Biomolecules offer several advantages as building blocks, which are highlighted here:

- Simple biomolecules, including amino acids, nucleobases, sugars, and others, are readily and naturally available in quantities and at prices amenable to preparing bulk quantities of materials.
- Biomolecules can lead to biologically-compatible MOFs.
- Biomolecules are structurally diverse. They can be either structurally rigid or flexible, aspects that impact the functional nature of the resulting MBioF.
- Biomolecules can have many different metal-binding sites. Consequently, they can exhibit multiple possible coordination modes, a feature that increases the potential structural diversity of MBioFs.
- Many biomolecules have intrinsic self-assembly properties which can be used to direct the structure and function of MBioFs.
- The ability of some of these biomolecules, specially in the case of nucleobases, to establish strong complementary hydrogen bonding favors the formation of open structures based on supramolecular non-covalent interactions (*supra*MBioFs).
- Finally, many biomolecules are chiral. Therefore, they can be used to construct chiral MBioFs, which may have interesting recognition, separation, and catalytic properties.

This suite of characteristics renders biomolecules particularly attractive building blocks for constructing MOFs with new properties and applications that cannot be accessed using the simple organic linkers traditionally used in MOFs construction.

Materials for Energy

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KEY WORDS: batteries, fuel cells, electrolytes.

The preparation of component materials for fuel cells and Li-ion batteries constitutes a research topic with great economic potential and social impact. Hence, the target of this research is threefold:

- The preparation of $\text{Ln}_{1-x}\text{A}_x\text{Fe}_{1-y}\text{M}_y\text{O}_3$ (Ln = lanthanide, A = alkaline earth metal, M = transition metal) and $\text{LnAB}_2\text{O}_{5+x}$ (Ln = lanthanide; A = alkaline earth metal; B = Cr, Fe, Ni, Co, Cd, Mg) type mixed oxides with perovskite structure for their use as electrodes in fuel cells.
- The preparation of potential candidates for electrodes in Li-ion batteries including Li and transition metal oxoanions (like phosphates, fluorosulphates, etc) and Fe or Co oxides.
- The development of safer and more reliable electrolytes to replace the currently used organic carbonate liquid solutions in batteries. The use of a solid electrolyte eliminates the need for containment of the liquid electrolyte, which simplifies the cell design, as well as improves safety and durability. There are two general classes of materials used for solid electrolytes: ceramic and polymer electrolytes .

Those materials will be synthesized at the nanoscale, thus, synthetic strategies will need to be optimized in order to be able to obtain homogeneous and monodispersed samples. Size reduction usually implies an electronic and structural reorganization of a compound and hence its properties will frequently be different from those observed in the bulk.

LITHIUM-ION BATTERIES

Lithium-ion batteries have arisen as one of the most promising technologies that can face the energy challenge in today's world. Our research is mainly focused on the obtaining of nanostructured materials. The best performing materials are then assembled as button-type cells and prototypes for their testing

SOLID OXIDE FUEL CELLS

Fuel cells are one of the most promising devices for environmentally clean power generation by converting chemical energy directly into electrical energy. In recent years, it has been further realized that the special micro/nanostructures could also notably influence the performance of materials.

ELECTROLYTES FOR BATTERIES

The electrolyte is the key component of any battery. Ceramic electrolyte membranes are one of the most promising breakthroughs in less-expensive and more durable materials. On the other hand, polymer electrolytes could be obtained as coatings and sheets, thus providing large area devices with integrated electronics. The conductivity of polymer electrolytes can be increased by improving the pore structure or adding ceramic nanoparticles.

Magnetic Materials.

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KEY WORDS: mixed oxides, *mixed oxides*, geometrically frustrated pyrochlore oxides, phosphates and phosphites of transition metals, functionalized nanoparticles, magnetism.

The present research line, which, in general terms, could be classified within the field of Materials Science, is focused on the synthesis and physicochemical characterization of three different families of compounds with potential technological applications: mixed oxides, phosphates and phosphites of transition metals and functionalized nanoparticles, which present applications in areas as conductivity, as potential components of SOFC's or medical therapy. The projects rely on the strong expertise developed by our group in the synthesis of novel materials - either in the solid-state (ceramic, freeze-dry, hydrothermal, ... methods) or in dissolution (sol-gel, microemulsion, polyol, ...) - and their subsequent characterization by spectroscopic techniques (EPR, UV-visible), microscopy (TEM, SEM.), diffraction (both x-ray and neutron), dc-magnetization and μ SR spectroscopy.

Mixed oxides of general formula $\text{Ln}_{1-x}\text{A}_x\text{M}_{1-y}\text{M}'_y\text{O}_3$ (Ln = lanthanide; A = divalent cation; M = Mn, Fe; M' = transition metal) with perovskite-type structures can display unusual magnetic properties (e.g. exchange bias). Double perovskites of general formula $\text{A}_2\text{BB}'\text{O}_6$ (A = lanthanide or alkaline-earth; B y B' = transition metals) are also attracting a great deal of interest as they can present large negative magnetoresistance combined with high Curie temperatures, which makes them suitable candidates for technological applications.

Parallel to this work on TM mixed oxides, our group has recently started a further line on the magnetic behaviour of pyrochlore oxides of formula $\text{RE}_2\text{M}_2\text{O}_7$ (with M = Ti, Sn, Ir, ...). Due to the low connectivity of the lattice, magnetic pyrochlores constitute the epitome of geometrical frustration. Once the energy scale of exchange coupling is removed by frustration, it is the balance of lesser terms in the spin Hamiltonian that determines the magnetic ground state of the system with crystal field anisotropy in particular playing a key role. Several systems have been studied by our group; among them, $\text{Pr}_2\text{Sn}_2\text{O}_7$, where non-conventional spin ice behaviour has been uncovered and $\text{Yb}_2\text{Sn}_2\text{O}_7$, with glassy behaviour below 150 mK despite what appears to be onset of long-range antiferromagnetic order.

Size confinement to a nanometer scale has induced effects not observed in macroscale. That is the case of magnetic properties, which are often remarkably different from those of their bulk counterparts. In this sense the third line of the research is centred on the superficial functionalization of Pd, PdFe, Fe_3O_4 and Fe_2O_3 NPs. The purpose is twofold: on the one hand, the functionalization alters the surroundings, and thus the electronic structure, of the metal atoms in the cluster, which changes their magnetic behaviour and, on the other, it allows the application of these particles in biological media. Most importantly, by optimization of complex synthetic methods in solution, our group has been able to prepare Pd-NR NPs with intrinsic ferromagnetic behaviour. Therefore, Pd magnetic nanoparticles could play an important role not only in the understanding of magnetism at nanoscale but also in the application in magnetic devices or in the biomedical field. The functionalization of magnetite NPs with different surfactants lets them to be manipulated by an external magnetic field, which opens up many applications involving the transport and/or immobilization of the nanoparticles. Finally, superparamagnetic nanoparticles have also been developed for use as contrast agents in both standard and functional MR imaging.

Organocatalysis: New Synthetic Methodologies towards Sustainable Chemistry

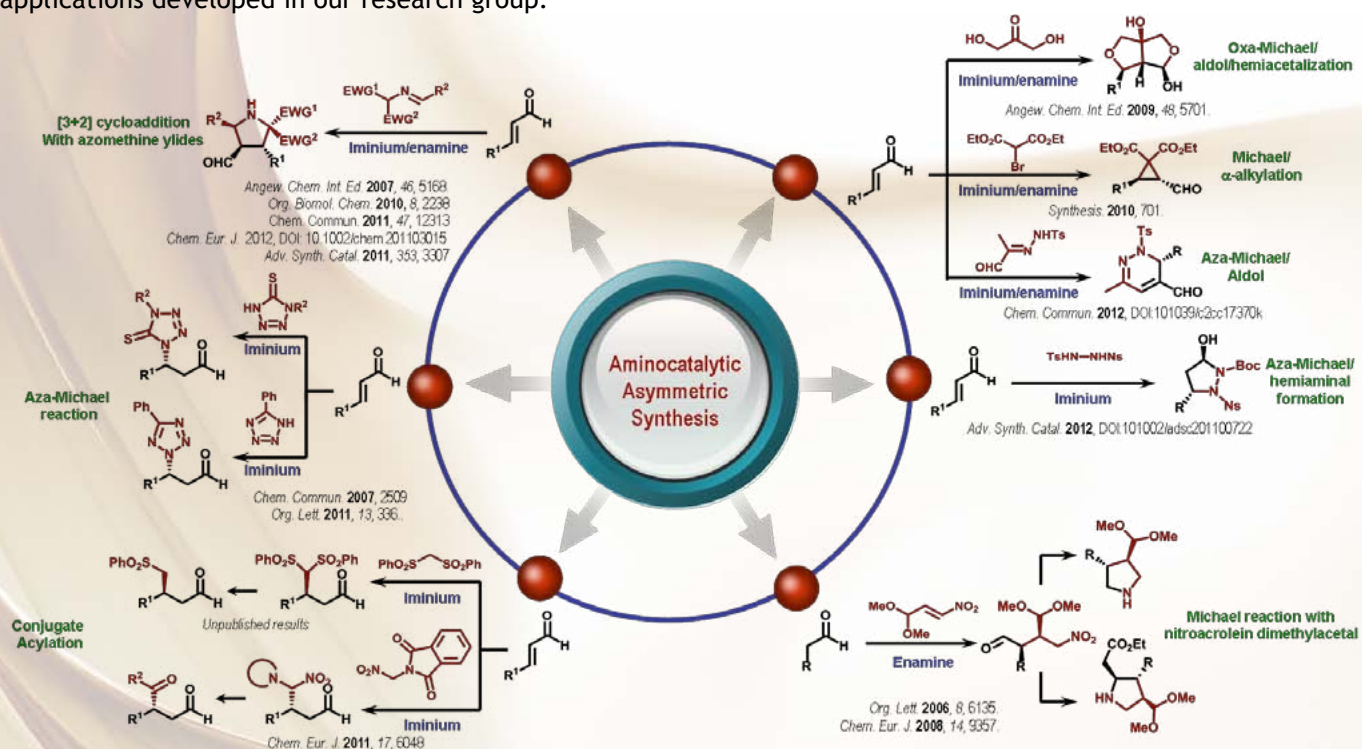
Jose Luis Vicario,* Luisa Carrillo, Efraím Reyes, Uxue Uria, Naiara Fernández, Maitane Fernández, Garazi Talavera, Jose Ignacio Martínez, Iratxe Ugarriza, Ane Orue, Iker Riaño, Laura Villar
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KEY WORDS: Organocatalysis, Green Chemistry, Chiral drug synthesis, Asymmetric Catalysis

Observing how Mother Nature solves complex problems in an easy way, the human being has been trying to imitate it for many centuries. Thus, the high catalytic efficiency of several enzymes in many natural processes has inspired many researchers to imitate and even improve its action, creating new protein-based biocatalysts. However, these show a rather narrow scope due to the inherent specificity of the biologic processes. For this reason, new and more flexible catalytic systems are needed for fine chemical production.

In asymmetric synthesis, not only should the catalyst accelerate the reaction but it also should be very stereoselective and flexible, in order to allow its use for the synthesis of different target molecules. In the last decade, organocatalysis has emerged as a very efficient tool in organic synthesis using small chiral organic molecules, which activate both reagents and reactants responsible for the stereocontrol of the reaction, in the absence of any metal. These organocatalysts are stable in air, water-compatible and easily prepared in both enantiomeric forms. Furthermore, most of them are commercially available, showing a great advantage when employed by pharma- and agrochemical industry, due to the fact that the presence of traces of contaminating transition metals is absolutely forbidden by legal regulations, avoiding additional purification methods.

Our research in this field has prompted us to study several organocatalytic methodologies and to the design of new catalysts which allow to carry out the reaction *in water*. These findings, together with the previously described advantages of organocatalysis compared to traditional metal catalytic reactions, are in accordance with the principles of *Green Chemistry*. Some of the following examples show the utility and the synthetic applications developed in our research group.



Our experience in Asymmetric Synthesis is well known and internationally recognized. Our research group provides laboratory facilities for students in the last year of degree, Master students, PhD. students or post-doctoral researchers. More information can be found in the group web page (<http://www.ehu.es/GSA>).

Organometallics in Synthesis

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KEY WORDS: asymmetric synthesis, organometallics, heterocycles

Our group works on Organic Synthesis, mainly in asymmetric synthesis and organometallic chemistry. Our projects are focused on the development of new synthetic methods of heterocyclic systems based on lithium, palladium, and ruthenium chemistry for the stereocontrolled formation of carbon-carbon bonds. The group has a solid background in Organic Synthesis, which allows us to face the preparation and structural determination of any kind of organic molecules.

Our research interests are summarized in the following lines:

Line 1. Metalation-cyclization sequence in the stereocontrolled synthesis of nitrogen heterocycles

The Parham-type intramolecular carbolithiation reactions for the construction of fused indolizidine and quinolizidine, and tetrahydroquinolines is explored, in order to determine the limitations and scope of the method. The diastereoselectivity of this metalation-cyclization sequence for the construction of non-planar systems, as well as its enantioselectivity, is studied performing the reactions in the presence of chiral catalysts or ligands.

Line 2. New applications of transition metal catalyzed reactions in the synthesis of fused indolizidines, quinolines, and homologues.

We are also developing new synthetic routes to natural products and analogues, which possess interesting biological activity, via palladium and ruthenium catalyzed processes. The intramolecular C-H activation reaction or direct aryl-aryl coupling is an interesting alternative to cross-coupling reactions in the formation of biaryl bonds on (hetero)aromatic systems. Both the direct arylation and the Mizoroki-Heck reactions use similar palladium-based catalytic systems, so the control of the chemoselectivity on polyfunctionalized substrates would allow the synthesis of different heterocyclic systems with interesting biological properties. Also strategies based on carbolithiation, direct arylation and Heck cascades are developed for the synthesis of polycyclic systems.

Line 3. Enantioselective alpha-amidoalkylation reactions

The Parham cyclization-enantioselective intermolecular alpha-amidoalkylation and organolithium addition-enantioselective intramolecular alpha-amidoalkylation sequences provide a novel synthesis of enantioenriched substituted fused isoquinoline systems. The enantioselection is controlled by using sterically demanding Brønsted acids as catalysts.

For reviews on our work, see: *Curr. Org. Chem.* **2003**, *7*, 275; *Eur. J. Org. Chem.* **2011**, 3610; *Carbolithiation of carbon-carbon multiple bonds*, in *Science of Synthesis. Knowledge Updates 2011/4*, D. G. Hall, K. Ishihara, J. J. Li, I. Marek, M. North, E. Schaumann, S. M. Weinreb, M. Yus, Eds.; Thieme: Stuttgart, **2012**, pp. 191-251.

For some selected publications: *Synlett* **2008**, 3188; *Org. Lett.* **2009**, *11* 1237; *Adv. Synth. Catal.* **2009**, *351* 2460; *J. Org. Chem.* **2012**, *77*, 2986.

More detailed information can be found in our web page: www.ehu.es/oms

Development of new methodologies for the synthesis of heterocyclic compounds

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KEY WORDS: Sustainable chemistry, Catalysis, Hypervalent iodine.

The two main research lines that are being conducted by our group are focused on the development of new synthetic methodologies to be carried out under sustainable conditions ("green chemistry").

• NEW METAL CATALYSTS: DESIGN AND APPLICATIONS

We plan to design and synthesize new catalysts -mainly based on palladium, copper or iron- to be used in tiny amounts under sustainable conditions (aqueous or biodegradable media, possible reuse of the catalyst...). Our preliminary research shows excellent results for a variety of transformations as shown in Figure 1. The described optimized methodology has allowed us to prepare a number of polycyclic compounds of interest (see Figure 2) with the benefits of short synthetic sequences, economical advantages, and sustainability when compared to previous reported alternatives

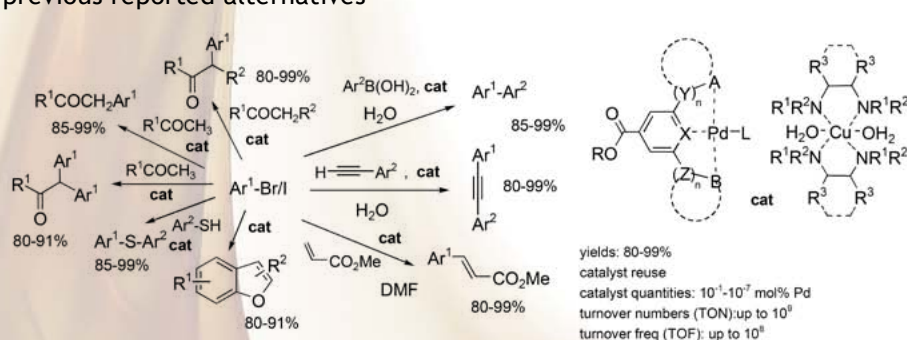


Figure 1. Selected reactions in which the new catalysts have been tested.

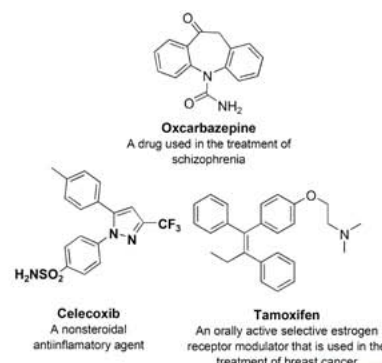


Figure 2. Target compounds prepared by the aid of the new catalysts.

• NEW APPLICATIONS OF THE HYPERVALENT IODINE REAGENT PIFA

PIFA, [bis(trifluoroacetoxy)iodobenzene], has become a prominent reagent in our ongoing synthetic plans due to the soft reaction conditions that are required, its high efficiency, and its low toxicity.

One of the most attractive features of this reagent involves its ability to oxidize properly substituted amides to generate highly electrophilic nitrenium intermediates. If under such conditions our starting material contains an internal nucleophile, a cyclic compound can be formed.

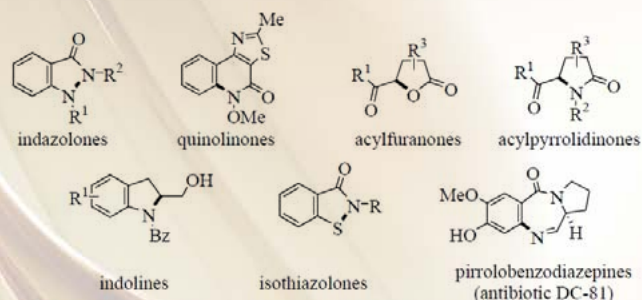
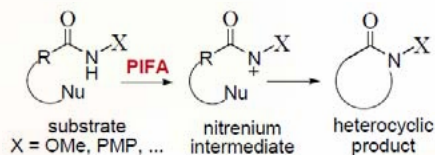


Figure 3. Selected examples of the use of PIFA in heterocyclic synthesis. The bond created by this reagent is highlighted.



The precise design of the substrates allows the preparation of a number of different heterocycles with high structural diversity (see Figure 3).



**Ingeniaritza Kimikoa/
Ingeniería Química**

Bio-refinery

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KEY WORDS: biomass, refinery, fuels, catálisis, chemicals, CO₂

OBJECTIVES

General. Development of catalytic processes for the sustainable production of fuels and chemicals from biomass.

Specific

- Design of catalysts, reactors and kinetic models for the reactions involved in biomass transformation.
- Development of new pathways for using CO₂ and CH₄ as raw materials in a bio-refinery.
- Development of tools for understanding the processes at multiple scales: from nanoscale (at the level of catalytic sites) to macroscale (designing pilot plants).

RESEARCH TOPICS

A. Selective production of olefins and aromatics from bio-oil, methanol and bio-ethanol. We are designing processes for the transformation of three key intermediates in the valorisation of biomass: (i) bio-oil from pyrolysis, (ii) methanol from gasification, and (iii) bio-ethanol from hydrolysis and fermentation. Furthermore, we are studying the compatibility of these oxygenates with hydrocarbons (from fossil fuels) and their co-processing in the same units.

B. Reforming of oxygenates (bio-ethanol, dimethyl ether) and bio-oil for hydrogen production. The reforming of pure oxygenates is currently being investigated in terms of (i) the design of enhanced catalysts, and (ii) the development of new kinetic models with a more accurate understanding of the reaction mechanisms. Concerning the reforming of untreated bio-oil, we have designed a new, original setup consisting of two steps in series to enable steady operation.

C. Using CO₂ as a raw material in the production of dimethyl ether. Dimethyl ether is an attractive fuel and intermediate in a bio-refinery. We investigate the following: (i) incorporating CO₂ as a raw material with syngas, (ii) developing new multifunctional catalysts, and (iii) designing enhanced reactors for reducing emissions and increasing selectivity.

D. Activation of methane for the production of olefins. Methane is an abundant molecule due to the increasing reserves of natural gas and its presence in biogas (produced from biomass, residues and wastes). We are developing a catalytic process for the transformation of chloromethane (obtained by chlorinating methane).

E. Intensification of propylene. Propylene is the olefin with the greatest market demand. However, refinery, bio-refinery and waste-refinery processes yield other olefins and paraffins that are in less demand. We study the conversion of surplus olefins and paraffins into propylene by designing new catalysts with enhanced activity and shape selectivity, and developing kinetic models for oligomerization-cracking steps.

F. Tackling catalyst deactivation in bio-refinery processes. In all the transformation processes involving oxygenates, wastes and residual feeds, the catalysts used undergo severe deactivation. The origin of this deactivation is mainly the deposition of hydrocarbons with lower H/C ratio than in the feed, namely, coking. We are researching the mechanisms and pathways of this deactivation and suggesting strategies that maximize the life of the catalyst and the viability of each process.

MORE INFORMATION: www.ehu.es/cpww

Waste-refinery

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KEY WORDS: wastes, plastics, tyres, refinery, fuels, energy, catalysis, chemicals

OBJECTIVES

General. Development of processes for the sustainable production of fuels and chemicals from wastes, and the upgrading of secondary streams in refineries.

Specific

- Development of processes towards the upgrading of highly aromatic refinery streams (LCO, PyGas, etc.).
- Incorporation into refineries of waste-derived streams, such as bio-oil, glycerol, sugars, plastics, waxes and tyre pyrolysis oil.
- Development of spouted bed technology. Hydrodynamic studies for its scaling up and industrial application (drying, combustion, pyrolysis and gasification).
- Thermal and catalytic processes for wastes (biomass, plastics, tyres, etc.) and secondary interest streams.

RESEARCH TOPICS

Sustainable refinery

A. Upgrading of aromatics by hydrocracking. Highly aromatic streams (residual streams), such as light cycle oil (LCO) and pyrolysis gasoline (PyGas) are under study via hydrocracking, in order to produce high value added fuels.

B. Upgrading of plastic wastes by hydroprocessing and cracking. Amongst the strategies studied, this section deals with the hydroprocessing (hydrogenation, hydrotreatment or hydrocracking) of waste plastics: 1) polyolefins (polyethylene and polypropylene) dissolved in other secondary refinery streams; 2) waxes and liquids produced in the pyrolysis of tyres, polyolefins or other plastics. In this manner, fuels with excellent properties for incorporation into current refinery schemes are produced.

C. Cracking and hydrocracking of renewable sources (oxygenates). Alternative routes are studied for cracking and hydrocracking bio-oil, glycerol and carbohydrates, which are by-products in the production of biodiesel and agricultural surplus.

Novel reactors and sustainable processes

D. Design, hydrodynamics and applications of spouted beds. The effect of internal devices on spouted bed hydrodynamics is studied in order to improve bed stability, scaling-up and treatment of different materials. This technology is being applied to the drying or combustion of granular materials.

E. Biomass pyrolysis, downstream catalytic cracking and gasification. The continuous pyrolysis of different types of biomasses is studied. Strategies for scaling up the process are developed: vacuum and autothermal pyrolysis. Furthermore, a two-step process has been set up for the upgrading of bio-oil and the production of high value added products: pyrolysis and downstream catalytic reforming. In addition, the production of syngas and hydrogen by steam gasification and their subsequent reforming is being studied.

F. Waste tyre upgrading by pyrolysis. Waste tyre upgrading by thermal and catalytic pyrolysis (HZSM-5, HY and H \square catalysis) is studied for the production of fuels and high value added products (limonene, isoprene).

G. Upgrading of plastic wastes by pyrolysis and gasification. The catalytic pyrolysis of polyolefins, polystyrene, PET and PMMA) is studied with the catalyst placed both in situ and downstream. These processes pursue the selective production of light olefins and fuels. In addition, steam gasification for the production of H $_2$ and syngas is studied.

MORE INFORMATION: www.ehu.es/cpww

Chemical Technologies for Environmental Sustainability

I. Prevention and control of pollutants from transport emissions and industrial effluents

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KEY WORDS: catalysis, depollution, depolymerization, dioxine, environmental, furane, green chemistry, incineration, NOx, recalcitrant contaminants, VOC, water treatment, zero emission.

The TQSA (Tecnologías Químicas para la Sostenibilidad Ambiental) team is focused to the *advancement in knowledge and enhancement of technologies applied to the protection of the environment and to the promotion and design of sustainable chemical processes*. We are researchers involved on several research areas. Concrete objectives and planning of tasks are defined in the following six general fields: 1. Development of structured catalysts and reactors; 2. Catalysis for automobile exhaust gas control; 3. Catalysis for removal of recalcitrant pollutants in industrial effluents; 4. Catalysis for energy production; 5. Future technologies for recycling and plastic waste resource management; 6. Environmental public health.

In this part I, content and projects under development in the three first above fields are summarized. The rest will be presented in part II.

1. DEVELOPMENT OF STRUCTURED CATALYSTS AND REACTORS

1.1. MONOLITHIC CATALYSTS. With more than 20 years of expertise in the preparation of cordierite monolithic catalysts (TWC, three-way catalysts), at present TQSA is involved in new applications for cordierite monoliths as De-NOx systems for diesel engine exhaust gas control, and in the development of "integral zeolite-based monoliths" (our patents EP 2412672 A1 and US 13/260.442) for combined NSR-SCR (see 2.2) and dDinOX (see 3.2).

1.2. METALLIC MICROSTRUCTURES AS CATALYTIC SUPPORT AND MICROREACTORS. These new structures can provide channels as small as 500 µm, which allows the miniaturization of reactors when the space is limited, e.g. "in situ" generation and purification of hydrogen for automobile fuel cells (see 3.2).

1.3. MATHEMATICAL MODELLING OF REACTION NETWORKS AND SIMULATION OF REACTORS. Mathematical models are being developed which fit experimental reaction data. Simulation of new environments and operation conditions with those models allow us to improve efficiency, or even to infer new systems or running conditions.

2. CATALYSIS FOR AUTOMOBILE EXHAUST GAS CONTROL

2.1. ADVANCEMENT IN CONVENTIONAL Pt-BaO/Al₂O₃-Monolith FOR DIESEL De-NOx. We have already developed the NSR (NOx storage and reduction) formulation, which fulfil requirements of Euro 5 emission standards (0.18 g/km), and now we are improving formulations for new Euro 6 regulations (0.08 g/km) to be applied in 2014.

2.2. COMBINED NSR-SCR SYSTEMS WITH INTERNAL PRODUCTION OF AMMONIA. We are trying to run the NSR system at such conditions in which the internal production of ammonia is optimized for stoichiometric reaction with NO slipping the NSR catalyst over a downstream NOx-SCR (selective catalytic reduction) which we are developing.

3. CATALYSIS FOR REMOVAL OF RECALCITRANT POLLUTANTS

3.1. REMOVAL OF VOC (Volatile Organic Compounds) AND METHANE FROM INDUSTRIAL EFFLUENTS. We are developing new formulations, substituting those based in noble metals, with less expensive redox materials, such as mixed oxides or manganese, cobalt oxides, with high activity, selectivity and durability.

3.2. SIMULTANEOUS REMOVAL OF NOx AND PCDD/PCDF FROM SOLID WASTE TREATMENT PLANTS (dDinOX). We are designing an integrated catalytic system zeolite-based with V₂O₅-WO₃ and/or Fe, able to remove simultaneously NOx, dioxine and furanes from urban solid waste incineration plant effluents. The reaction network is being investigated.

Chemical Technologies for Environmental Sustainability

II. Hydrogen for fuel cells, plastic waste recycling, and environmental public health

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KEY WORDS: air quality, catalysis, clean energy, depolymerization, emerging pollutant, environmental, hydrogenation, hydrocracking, polymer recycling, PROX, priority pollutant, reforming, water treatment.

The TQSA (Tecnologías Químicas para la Sostenibilidad Ambiental) team is focused to the *advancement in knowledge and enhancement of technologies applied to the protection of the environment and to the promotion and design of sustainable chemical processes*. We are researchers involved on several research areas. Concrete objectives and planning of tasks are defined in the following six general fields: 1. Development of structured catalysts and reactors; 2. Catalysis for automobile exhaust gas control; 3. Catalysis for removal of recalcitrant pollutants in industrial effluents; 4. Catalysis for energy production; 5. Future technologies for recycling and plastic waste resource management; 6. Environmental public health.

In the part I, content and projects under development in the three first above fields were summarized. In this part II the remaining three fields are presented.

4. CATALYSIS FOR CLEAN ENERGY PRODUCTION

4.1. HYDROGEN PRODUCTION BY REFORMING OF LOGISTIC FUELS. Oxidative reforming of simulated gasoline and gasoil streams with water vapour over nickel aluminate as the active phase is being investigated as catalysts with improved activity, selectivity and durability compared to more conventional rhodium catalysts.

4.2. CO REMOVAL FROM HYDROGEN FEEDSTREAMS FOR FUEL CELLS. The purification of hydrogen to be fed to PEM fuel cells is achieved by two consecutive reactions, WGS (Water Gas Shift) and CO-PROX (Preferential Oxidation). At present we are studying new catalyst formulations for a substitute single process, OWGS (Oxygen-enhanced WGS). The process should be carried out *on-board* in microreactors (see 1.2).

5. PLASTIC WASTE RESOURCE MANAGEMENT (RECYCLING AND VALORIZATION)

5.1. DEPOLYMERIZATION OF PLASTICS TO MONOMERS. We have studied PET depolymerization by alkaline hydrolysis using quaternary salts as catalyst. The glycolysis with ethylene glycol, in which we are now involved, allows the use of highly eco-efficient catalysts and the production of BHET (bis-2-hydroxyethylterephthalate), as raw material for a wide range of high value product synthesis.

5.2. HYDROGENATION AND HYDROCRACKING OF WASTE MIXED PLASTICS. The research is focused to mixtures of complex plastics as polystyrene (highly aromatic) or PVC (halogenated). Bifunctional metal-acidic catalysts are needed to carry out the process towards molecules suitable to be added to the gasoline-pool, and the process demands high pressure and intermediate temperature. Several kinetic models have been developed.

6. ENVIRONMENTAL PUBLIC HEALTH

This research is focused to the development of predictive tools for evaluation of health risk by mathematical modelling, optimal control of process variables in drinking water treatment plants, and development of new technologies to be implemented in tertiary water treatment, such as selective adsorption, membranes and catalytic oxidation. The following lines are open to research:

- Strategies for reduction of priority and emerging pollutants in drinking water treatment plants.
- Removal of nanoparticles by membrane filtration in aqueous effluents.
- Air quality monitoring and detection of black-points (PM₁₀, PM_{2.5}, NO_x, O₃, CO and SO₂) in the Basque Country.
- Control of diffuse air emissions by teledetection.



**Kooperatiba-
-Ikerketarako Zentroak/
Centros de Investigación
Cooperativa (C.I.C.)**

The Biophysics Unit: A joint CSIC-UPV/EHU research center for biophysical studies of biomembranes and other biological systems

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KEY WORDS: Biophysics Unit, Research Center, biophysics, biological systems, biomembranes.

The Biophysics Unit (Unidad de Biofísica) was created in 1999 and is a joint Center of the Universidad of the Basque Country (UPV/EHU) and the Spanish Science Research Council (CSIC). The Biophysics Unit has two main objectives: To carry out high-quality research studies in the field of biomembranes and other biological systems of current interest, and to educate young scientists according to international quality standards. The Center offers state-of-the-art equipment to perform innovative and multidisciplinary studies integrating areas such as physics, biochemistry, molecular and cellular biology, and computational biology. It currently hosts 91 researchers (Ph. D. students, post-doctoral fellows, and staff scientists) working in 16 different research groups. Below we show 4 representative research lines of our Center.

IONIC CHANNELS AND CELL EXCITABILITY (Alvaro Villarroel)

Our research is focused on the molecular study of ionic channels that regulate cell excitability. In humans, mutations of these proteins cause arrhythmia, epilepsy and deafness. Our objective is to identify the network of regulatory factors (proteins and lipids) associated with these membrane proteins, by analyzing the physiological consequences of these interactions through mutagenesis-function studies, and the use of electrophysiological, imaging, biochemical and high-resolution biophysical techniques.

MITOCHONDRIAL MEMBRANES, APOPTOSIS AND CANCER (Gorka Basañez)

During apoptosis, mitochondrial membranes undergo dramatic changes in permeability and morphology. The principal components involved in these processes are the BCL-2 family proteins, with the assistance of an increasing number of protein/lipid effectors. We use a multidisciplinary approach based on biophysical techniques to try elucidating the mode of action of these mitochondrial membrane components at the molecular level. Considering the important role played by BCL-2 family proteins in tumorigenesis and the cellular response to chemotherapy, the information gained may facilitate progress in the fight against cancer.

STRUCTURAL GLYCOBIOLOGY (Marcelo Guerin)

Glycans are not only one of the major components of the cell but also modulate a variety of important biological processes in all living organisms. Most of the enzymes responsible for the biosynthesis of glycan structures are glycosyltransferases. The long-term goal of our research program is to understand how glycosyltransferases function to control health and disease at the molecular level. To this end, we are using a multidisciplinary approach including molecular biology, protein biochemistry/biophysics and structural biology.

MEMBRANE PROTEIN FOLDING AND STABILITY (Ana Rosa Viguera)

Protein folding has been the subject of intensive research. Combinations of experimental and computational studies are enabling folding to be followed at atomic resolution, with the result that general rules are emerging. This insight, however, mainly pertains to water-soluble proteins and it is unclear whether the emerging mechanisms extend to the many proteins that reside in membranes. We investigate the kinetics and thermodynamics of folding aiming to obtain mechanistic detail on membrane α -helical proteins. We have chosen the pore-forming fragment of colicin A (ColA) as a model to study protein-lipid complex formation and stability.

NanoGUNE, the big challenge of the small

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KEY WORDS: nanoscience, nanotechnology, training, education.

The CIC nanoGUNE Consolider has the mission of addressing basic and applied world-class research in nanoscience and nanotechnology, fostering high-standard training and education of researchers in this field, and promoting cooperation among different agents in the Basque Science, Technology, and Innovation Network (Universities and Technological Centers) and between these agents and the industrial sector.

NanoGUNE is one of the main pillars of the nanoBasque Strategy, launched by the Basque Government in 2008 to promote the competitiveness of the Basque Industry through the incorporation of nanotechnology.

NanoGUNE is a non-profit association that includes UPV/EHU, the Donostia International Physics Center, Tecnalia, IK4, and the Regional Council of Gipuzkoa.

The Molecular Imaging Facility at CIC biomaGUNE

CIC biomaGUNE

Paseo Miramón, 182, 20009 Donostia-San Sebastián (Gipuzkoa)

The Molecular Imaging Facility at CIC biomaGUNE is housed within 900 m² and is an integrated imaging facility that offers state-of-the-art resources in Radiochemistry, Positron Emission Tomography (PET), Single Photon Emission Computerized Tomography (SPECT), Computerized Tomography (CT), Magnetic Resonance Imaging (MRI) and Optical Tomography (OT). Including a dedicated Animal Housing Facility for rodents, the Molecular Imaging Facility has been created with the aim of becoming a reference research centre in Europe in the field of Molecular Imaging in small animals.

RADIOCHEMISTRY

The Molecular Imaging Facility is equipped with an IBA Cyclone 18/9 cyclotron with seven targets for the routine production of [¹⁸F]F- (2 units), [¹⁸F]F₂, [¹³N]NH₄⁺, [¹⁵O]O₂, [¹¹C]CO₂ and [¹¹C]CH₄. A solid target suitable for the production of other positron emitters (e.g. ¹²⁴I, ⁸⁹Zr, ⁴⁵Ti) and a ⁶⁸Ga generator are also available. In the Radiochemistry Laboratory, 6 large hot cells house automated synthesis modules for the production (including synthesis, purification and formulation) of PET and SPECT radiotracers.

NUCLEAR IMAGING

The Nuclear Imaging area is equipped with one eXplore speCZT SPECT-CT (axial FOV = 80 mm, trans-axial FOV = 32 mm for mouse and 76 mm for rat) and one eXplore Vista PET-CT (axial FOV = 47 mm, trans-axial FOV = 67 mm) for in vivo imaging.

MAGNETIC RESONANCE IMAGING

The MRI Laboratory is equipped with an actively-shielded ultra-refrigerated superconducting 11.7 Tesla magnet, operating at a proton resonance frequency of 500MHz, interfaced to a modern Bruker Avance system to enable: i) High resolution anatomical imaging in 2D or 3D; ii) Functional MRI; iv) Volume selective spectroscopy and spectroscopic imaging methods (¹H, ¹³C, ¹⁹F and ³¹P). Optimized ancillary equipment for animal positioning, monitoring and triggering are used to ensure animal welfare during scanning.

OPTICAL IMAGING AND AUTORADIOGRAPHY

As a complement to nuclear and magnetic resonance imaging systems, a high sensitivity optical tomograph equipped with X-ray imaging has been installed in the Nuclear Imaging Area. A digital autoradiography system (FOV of 200 x 250 mm) to perform ultrafast and quantitative ex vivo studies with spatial resolution in the micro scale is also available.

ANIMAL HOUSE

The dedicated Animal Facility has been designed with two different areas: an animal acclimatization area, and an experimental area.

Research at CIC BIOMAGUNE

CIC biomaGUNE

Paseo Miramón, 182, 20009 Donostia-San Sebastián (Gipuzkoa)

CIC biomaGUNE (<http://www.cicbiomagune.es>) focuses its activity in the fields of Nanobiomaterials and Molecular Imaging and is presently constituted by three Research Units:

Biofunctional Nanomaterials Unit

The design, the construction and the characterization of biofunctional nanostructures that can readily interact with biomolecules both on the cell surface and within the cell constitute the main research topic of this Unit.

Research Groups:

Prof. Soledad Penadés.- This laboratory has established a methodology to construct well defined water soluble three-dimensional carbohydrate polyvalent model systems (glyconanoparticles) as a tool for the study of biologically relevant interactions.

Recent publications: *Biomaterials* **2011**, *32*, 9818; *Chem. Eur. J.* **2011**, *17*, 1547; *Bioconjugate Chem.* **2011**, *22*, 264.

Dr. Niels-Christian Reichardt.- This laboratory is mainly devoted to the preparation of microarray-based tools for studying protein-carbohydrate interactions of biomedical or industrial importance.

Recent publications: *Angew. Chem. Int. Ed.* **2011**, *50*, 1801; *J. Am. Chem. Soc.* **2011**, *133*, 1695; *Chem. Commun.* **2011**, *47*, 2390.

Dr. Valery Pavlov.- This laboratory deals with the preparation of artificial complex biochemical systems (multicomponent biocatalytic systems, signal-responding biosystems, self-organizing / self-structuring functional biosystems) for biomedical applications.

Recent publications: *Biosens. Bioelectron.* **2011**, *30*, 272; *Analyst* **2010**, *135*, 2291; *Chem. Eur. J.* **2010**, *16*, 6187.

Dr. Juan C. Mareque.- The main research topic in this laboratory is the design, the preparation and the study of inorganic complexes and nanomaterials for a range of medical applications.

Recent publications: *Chem. Commun.* **2011**, *47*, 2995; *Mol. Biosystems* **2010**, *6*, 1572; *Angew. Chem. Int. Ed.* **2009**, *48*, 356.

Biosurfaces Unit

The design and build up of biofunctional nanosurfaces on different supports to investigate relevant problems in biology and to understand and predict the interactions of living cells with materials constitute the general research topic of this Unit.

Research Groups

Dr. Ilya Reviakine.- Research in this laboratory is centred around interfaces between inorganic materials and soft self-assembling biologically relevant materials.

Recent publications: *Anal. Chem.* **2011**, *83*, 8838; *Anal. Chem.* **2009**, *81*, 8167; *Langmuir* **2009**, *25*, 5177.

Dr. Sergio E. Moya.- The research in this laboratory focuses on nanofabrication and on the study of the properties of nanostructured biomaterials.

Recent publications: *Macromol. Rapid Commun.* **2011**, *32*, 1972; *Nanoscale Res. Lett.* **2011**, *6*, 429; *Soft Matter* **2011**, *182*, 208.

Dr. Ralf Richter.- This laboratory is dedicated to the study of self organization and dynamic supramolecular assembly of lipid membranes and the polysaccharide-rich pericellular coat.

Recent publications: *Anal. Chem.* **2011**, *83*, 8838; *J. Biol. Chem.* **2011**, *286*, 25676; *Int. J. Mater. Res.* **2011**, *7*, 6883.

Molecular Imaging Unit

Research in this Unit is mainly devoted to develop new products and methodologies to study relevant biomedical problems in vivo using molecular imaging technologies.

Research Groups:

Dr. Jordi Llop: Research in this laboratory is focused on the development of new imaging agents with potential application in Positron Emission Tomography (PET) and Single Photon Emission Tomography (SPECT).

Recent Publications: *J. Nucl. Med.* **2011**, *52*, 526; *Nucl. Med. Commun.* **2011**, *32*, 1011; *Neuroscience* **2011**, *182*, 208.

Dr. Torsten Reese.- Research in this laboratory is mainly centred in the utilization of optimized Magnetic Resonance (MR) methods to relate pathophysiology to function in various animal models.

CIC Energigune Energy Cooperative Research Center. Materials for Energy Storage

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KEY WORDS: energy storage, batteries, supercapacitors, heat storage.

CIC Energigune is a new energy research centre with headquarters in the Basque Country that aims to become an international benchmark in its field. The centre has two main research areas: Power Storage, Batteries and Supercaps (PSBS) and Thermal Energy Storage (TES) and has the backing of public institutions, administrations, and of companies directly related to the energy sector.

CIC Energigune is focused on basic oriented research on energy related technologies, aimed at improving materials for energy storage systems focused on renewables and power applications. Both PSBS and TES research areas have the support of an Electron Microscopy (EM) Platform, a Surface Analysis Unit, an X-ray Diffraction Platform and a Solid State Nuclear Magnetic Resonance (NMR) Platform all of them also open to external users. It is noteworthy to mention that the infrastructure includes (i) a 200kV field emission gun (FEG) high resolution TEM/STEM, (ii) a high resolution low-vacuum FEG SEM, (iii) a multi technique multi chamber UHV Surface Analysis System for X-ray Photoelectron Spectroscopy (XPS), Auger Electron Spectroscopy (AES), SEM/SAM and depth profiling, (iv) a small-angle X-ray scattering (SAXS) instrument and (v) two wide bore solid state NMR instruments equipped with 200 MHz and 500 MHz superconducting magnets that can reach spinning speeds up to 65 kHz.

In the field of PSBS the main research lines are:

- **Na-ion batteries**, oriented to the synthesis and characterization of both cathode and anode materials.
- **Li-air batteries**, focusing on the development of nanoarchitected air cathodes and on the synthesis of hybrid organic-inorganic nanocomposite anode materials.
- **Solid electrolytes**, which comprehends the synthesis and characterization of ceramic and polymer electrolytes both for Li-ion and Na-ion batteries.
- **Supercapacitors**, centered on the optimization of electrochemical double-layer capacitors (EDLC's) and pseudocapacitors through tailoring electrode materials.

In the area of TES the research is focused on:

- **Latent heat storage**, focused on the development of new phase change materials at medium-to-high temperature range.
- **Sensible heat storage**, where the storage of energy by sensible heat process, using liquid or solid materials, is studied.



**Beste proiektuak/
Otros proyectos**

UNIVALUE PROJECT

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Local contact José Manuel Pérez Arce

KEY WORDS: Valuation, Commercialization, Transfer, Patent, Technology, Knowledge.

The universities are aware of the difficulty in bringing the results of university research into the socio-economic realm. Promoting Excellence in Research and Transfer of Results should be pointed out as their primary objectives. **UNIVALUE VALORIZACIÓN S.L.** was founded to facilitate valuation (appraisal) of the results obtained by G9 and their transfer to the market. The expertise of a highly specialized team for **Valuation (Appraisal) and Transfer of Technologies and Knowledge** will accomplish this facet.

Grupo G9 de Universidades (www.uni-g9.net) is constituted by the following universities: Universidad de Cantabria, Universidad de Castilla La Mancha, Universidad de Extremadura, Universitat de les Illes Balears, Universidad de La Rioja, Universidad de Oviedo, Universidad del País Vasco (UPV/EHU), Universidad Pública de Navarra y Universidad de Zaragoza.

BUSINESS AREAS:

- Agriculture Industry
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- Chemistry
- Civil Engineering
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- Mechanical Engineering
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- Environment and Natural Resources
- Health & Safety
- Healthcare and well-being
- Legal Sector
- Leisure, Culture and Education
- Management Technology
- Materials
- Metallurgy
- Music
- Physics
- Renewable Energy
- Robotics
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UNIVALUE VALORIZACIÓN S.L. focuses on two different but complementary activities:

- **VALUATION (appraisal)** of Patents and Technologies.
- **COMMERCIALIZATION (marketing)** of Patents and Technologies.

UNIVALUE has a team of professionals highly qualified in technology as well as in marketing. The competent team has been selected to handle the present and future demands of the different aspects of Knowledge coming from the Universities. Enclosed an example of two Technologies ready to transfer.

REF: TC 07047

FICHA TÉCNICA

UNIVALUE VALORIZACIÓN Y TRANSFERENCIA TECNOLÓGICA G9 ACTION

PRODUCTO DE LIMPIEZA NO ABRASIVO PARA LA PIEDRA.
Tecnología de limpieza de contaminantes, biofilms y grafitis de fachadas y piedra monumental, mediante tratamiento con resina.

I. Limpieza de la piedra monumental
El humo del tráfico, la contaminación atmosférica, los grafitis...son sólo unos pocos ejemplos de todos los factores externos que pueden ensuciar las fachadas y monumentos de piedra caliza de nuestras ciudades y pueblos.
Ahora posible efectuar una **limpieza profunda y no agresiva** gracias a esta tecnología basada en resinas que actúa a modo de peeling eliminando todo resto orgánico e inorgánico de la superficie de la piedra sin dañarla.
Toda piedra con **alto contenido en carbonatos** puede ser limpiada mediante este tratamiento.

II. Ventajas competitivas
Actualmente de limpieza de la piedra caliza se realiza con agresivos métodos tales como el chorro de arena que atacan físicamente por lo que conlleva una pérdida importante de material.
La **gran ventaja** de este nuevo producto es que la limpieza se basa en una **reacción química** entre la piedra y la resina **sin dañar** la piedra.
De fácil aplicación y respetuosa con el medio ambiente, esta **Green Technology** no produce residuos tóxico ni es peligrosa para el ser humano.

III. Aplicaciones
Esta tecnología ha sido probada con éxito en la recuperación de un retablo de iglesia de piedra caliza. Así mismo, se está probando actualmente en fachadas de edificios urbanos.
Los tipos de piedra susceptibles de ser protegidos con esta tecnología son, entre otras:
• Piedra caliza
• Arenisca carbonatada
• Cemento
• Piedra Dorada de Baeza
• Mármol

IV. Dirigido a...
El mercado final de la tecnología abarca todo tipo de empresas que presten sus servicios de conservación y limpieza de la piedra tanto a Organismos Públicos como a particulares.
Este producto para la limpieza de piedra con base carbonatada, está preparado para ser utilizado en el sector de la **Conservación del Patrimonio Monumental** (edificios emblemáticos) y en todo tipo de piedra o material con base carbonatada.

V. Saber más
Esta tecnología cuenta con el respaldo científico y técnico de un prestigioso equipo de investigación del Grupo G9 de Universidades, Grupo puntero en desarrollo tecnológico Español.
Esta tecnología cuenta con el amparo de la Ley 16/1985, de 25 de Junio del Patrimonio Histórico Español.

Piedra antes de la limpieza **Piedra después de la limpieza**

Si Ud. quiere disponer de más información sobre nuestro producto, consultenos sin compromiso.
Nuestros técnicos estarán encantados de atenderle. info@univalueg9.com / Tlf: +34 944 435 400 / www.univalueg9.com

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REF: TC 07046

FICHA TÉCNICA

UNIVALUE VALORIZACIÓN Y TRANSFERENCIA TECNOLÓGICA G9 ACTION

MICROCAPA PROTECTORA PARA MANTENIMIENTO DE LA PIEDRA.
Acondicionamiento para la protección de fachadas y piedra monumental mediante tratamiento con resina.

I. Conservación de la piedra monumental
Muchos países poseen un gran Patrimonio Monumental y fachadas de piedra caliza que requieren de un **mantenimiento** y protección periódicos.
Les presentamos un nuevo producto de conservación basado en una **microcapa** que actúa protegiendo la piedra sin variar su color ni las características estéticas tales como el brillo o la porosidad.
Toda piedra con **alto contenido en carbonatos** es perfecta para ser protegida mediante esta tecnología.

II. Ventajas competitivas
Los actuales métodos de conservación de la **piedra caliza** dejan una patina blanca que supone un cambio estético en monumentos y fachadas de piedra caliza entre otras.
La **gran ventaja** de este producto es que se basa en una reacción química entre la piedra y la resina **sin dejar capas ni brillos**.
Así mismo, este acondicionamiento no resulta agresivo para la piedra ya que no conlleva pérdida alguna de material.

III. Aplicaciones
Se han realizado con éxito diversas pruebas en edificios emblemáticos con fachadas de piedra con base carbonatada.
Los tipos de piedra susceptibles de ser protegidos con esta tecnología son, entre otras:
• Piedra caliza
• Arenisca carbonatada
• Cemento
• Piedra Dorada de Baeza
• Mármol

IV. Dirigido a...
El mercado final de la tecnología abarca todo tipo de empresas que presten sus servicios de conservación y protección de la piedra tanto a Organismos Públicos como a particulares.
Este producto para la conservación de la piedra está listo para ser utilizado en el sector de la **Conservación del Patrimonio Monumental**, edificios emblemáticos y en todo tipo de piedra con base carbonatada.

V. Saber más
Esta tecnología cuenta con el respaldo científico y técnico de un prestigioso equipo de investigación del Grupo G9 de Universidades, Grupo puntero en desarrollo tecnológico Español.
Esta tecnología cuenta con el amparo de la Ley 16/1985, de 25 de Junio del Patrimonio Histórico Español.

Resina base de la Tecnología

Si Ud. quiere disponer de más información sobre nuestro producto, consultenos sin compromiso.
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Euskampus Knowledge Poles

Building and Cocreating New Spaces of Collaboration to Tackle Global Challenges

KEY WORDS: Research, Innovation, Collaboration, Co-creation,

“There exists an inadequacy growing every day, deeper, more profound and more serious between on one side our articulated knowledge, parceled and compartmentalized, and on the other the realities of problems more and more multidisciplinary, cross-sectional, multidimensional, cross-national, global and planetary”, Edgar Morin.

The knowledge poles are in the heart of the Euskampus project and they have been designed, and thought as a strategic element that serves to concentrate and categorize all activities of the areas of education, investigation, innovation and transfer into each of the specializing areas: quality of life and healthy ageing, new materials and innovating processes, sustainable ecosystems and environmental technologies etc.

The launching of these Knowledge Poles begins with identifying the science-technological challenges, common among their partners' excellence investigation teams, UFI, GEI, Business Units, etc, according to the lines of specialization of Euskampus project

This work formula has the aim to become a methodology, establish the dynamics and set up the know-how, to make it last in time and allowing it to systematize the joint of collaboration networks between multidisciplinary teams, that belong to different organizations which take part in Euskampus Fundazioa.

Knowledge Poles advantages:

1. They are not functional nor organizational structures; they don't belong to any Euskampus member.
2. They favor the permeability of the different agents implied.
3. They promote the cross-section work among different organizations that usually work in “silos”. They optimize resources and pursue the maximum efficiency and effectiveness of the whole system.
4. The service and management of Euskampus Fundazioa, fast and flexible, to ease the investigation activity, erasing barriers and stiffness of the system, supplying or activating the necessary resources, speeding up and adjusting their accessibility to each moment of the project.

