

# Participant Abstracts

1a Jornada d'Investigadors Predoctorals Interdisciplinària

Universitat de Barcelona, February 7, 2013

## Session I. Theory

chairman: Blai Garolera

### 1. Xumeu Planells Noguera

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#### **Study of parity breaking in a hot/dense nuclear medium**

In this talk I will give a short introduction in particle physics: why it is important, what this discipline explores, how it is investigated, etc. Within the presented framework, the particle collisions produced in the widespread LHC (and similar machines) are the appropriate mechanism to study and understand the main constituents of matter. In particular, heavy ion collisions are convenient to create very hot and dense nuclear matter medium in order to extract information about the strong nuclear force (one of the four fundamental interactions of nature) and its phase diagram (thermodynamics). In such extreme conditions, nothing prevents the breaking of parity symmetry, one of the main properties of strong interactions (which can be associated to a mirror reflection). The hypothesis that a new phase with this feature could be reached in the LHC is not only interesting by itself, but also opens the possibility to explain some anomalous results that are seen in heavy ion collisions experiments.

*Keywords:* heavy ion collisions, QCD phase diagram, phenomenology, particle physics, thermodynamics of strong interactions, phenomenology

### 2. Daniel Fernández

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#### **Properties of holographic superfluids**

At extremely low temperatures, some fluids experience a phase transition, becoming what is called superfluids and displaying strange properties, such as almost zero viscosity. The holographic approach to the gauge theory that describes the superfluid phase enables us to reformulate the system in terms of a higher dimensional gravitational theory. An analysis of the spacetime geometry perturbations provides qualitative predictions about transport properties of the superfluids that may be measured in experiment.

*Keywords:* Gauge-gravity correspondence, Holography, Black Holes, Superfluids

### 3. Guillem Perarnau

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#### **Permutacions que eviten certs patrons**

En aquesta xerrada explicaré una nova aproximació pel problema de comptar permutacions que eviten un cert patró. Tradicionalment aquest problema ha estat atacat utilitzant eines de combinatòria algebràica. Aquest nou mètode permet donar proves més senzilles de resultats ja existents així com obtenir nous avenços en aquesta àrea.

*Keywords:* Permutació, Combinatòria, Patrons, Probabilitat

### 4. Marc Suñé Simon

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#### **Anomalous transport and diffusion of overdamped Brownian particles in totally disordered potentials**

Anomalies in both transport and diffusion phenomena have already been shown for non-interacting free Brownian particles in nonlinear potential landscapes. These anomalous behavior is enlightened when particles undergo a disordered potential. We have check the incidence of the disorder's correlation function and a constant external force on transport and diffusion of overdamped Brownian particles, in either one and two dimensions, by the numerical analysis of the Langevin equation.

*Keywords:* Brownian motion, transport, diffusion, disorder

### 5. Martí Perarnau Llobet

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#### **Work Extraction and Entanglement**

Consider a (quantum) battery which stores some energy. It may happen that, although it has energy, no work can be extracted fom the battery (for example, if it has a lot of entropy, i.e., disorder). One then says that the battery is in a passive state. Quite surprsingly, if we have more than one passive state, then work can be obtained. That is, work can be extracted globally although individually it is not possible. In this talk, I will explain why this is so and I will mention the role quantum entanglement may play.

*Keywords:* quantum, thermodynamics, work, entanglement

### 6. Elsa Passaro

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#### **Quantum correlations for information processing**

In the last decades, the distinguishing features of quantum theory have been exploited to accomplish tasks which are unfeasible in classical theory. One of the most important resources which has shown the advantages obtained compared to the classical setting is quantum entanglement. Entangled systems (i.e. composite quantum system whose joint state cannot be written in product form) are indeed essential for many quantum information processing protocols including teleportation, superdense coding, quantum computation and secure communication.

Recently, new protocols were proposed in the so-called device-independent scenario, where no assumption is made on the involved devices, but only correlations between preparations, measurements and outcomes are considered. The advantage offered by device-independent protocols is that they are extremely robust due to the weakness of the hypotheses on which they rely.

In this scenario, quantum correlations i.e., correlations which can result from local measurements on quantum states - play a central role in the certification of the quantum nature of a source as well as its dimensionality. Quantumness of correlations manifests, for instance, when any local complete projective measurement on a subsystem necessarily alters the state of a composite system. Such correlations are revealed by the violation of a suitable Bell inequality, which certifies the reliability of the considered protocol.

*Keywords:* quantum correlations, entanglement, device-independent, Bell inequality

## 7. Xavier Clotet i Forns

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### **The breakfast experiment: understanding kinetic roughening**

We study experimentally the kinetic roughening process of imbibition interfaces. Imbibition is a process of fluid transport in a medium in which the resident fluid is displaced by a second immiscible invading fluid that preferentially wets this medium. When this process occurs in a disordered medium the system develops long range correlations along the interface due to the competing forces acting on different length scales. As a result, the system evolves out of equilibrium towards a statistically stationary state with critical fluctuations of the interface. The dynamics is highly heterogeneous both in space and time. The roughened interfaces we get can be related to the ones observed in fracture processes or in the growth of bacterial colonies (or the contour of Montserrat mountain). The global dynamics of the front corresponds to crackling noise.

*Keywords:* Statistical physics, disordered media, kinetic roughening

## 8. Gonzalo de la Torre Carazo

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### **Do completely unpredictable events really exist in nature?**

Classical mechanics is a fully deterministic theory. This means that no intrinsic randomness really exists within the theory and all uncertainty in its predictions can be traced back to a lack of knowledge on the initial conditions of the physical phenomena. On the contrary, quantum mechanics makes predictions only in probabilistic terms, allowing for randomness within its axiomatic structure. This change of paradigm makes apparent that in order to answer whether completely unpredictable events really exist one should certify the randomness independently of the physical framework used. Bell tests approach the question from this perspective: Correlations between distant systems violating a Bell inequality are, assuming no instantaneous communication between the parties and the freedom of choice of the experimenters, incompatible with underlying deterministic explanation. However, the free choice of the experimenters assumption accounts for initial perfect randomness making the argument circular. In this talk I'll present recent works aimed at relaxing such assumption up to its breaking point. As a consequence, we will be left with a strict dichotomic choice of paradoxically indistinguishable worlds: either everything in our world is fully predetermined or there exist in nature events that are completely unpredictable.

*Keywords:* randomness quantum unpredictable deterministic Bell random

9. **Adriana Di Dato**

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**Black holes in higher dimensions**

The theory of general relativity predicts the presence of black holes. I will introduce them in a four dimensional space-time and I will show what happens if we increase the number of dimensions. It is possible to prove the existence of new types of black holes without any fourdimensional counterpart. Moreover, I will present an effective theory to study their dynamics and how I can treat a black hole as a fluid.

*Keywords:* black holes

10. **Alejandro Turpin Avilés**

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**Refracció cònica: fenomen i aplicacions**

La refracció cònica és un fenomen predit teòricament per Hamilton al 1832 que va ser fonamental en l'acceptació de la teoria ondulatoria de la llum i en el qual un feix col·limat de llum és transformat en un cilindre buit després de passar al llarg de l'eix òptic d'un cristall biaxial. Tot i ser un fenomen antic, la comprensió profunda del fenomen s'està produint en els darrers anys. Les propietats úniques del fenomen poden ser molt rellevants en camps com làsers, micro-manipulació, trampes atòmiques, comunicacions òptiques a l'espai lliure, etc.

*Keywords:* -

11. **Jose Manuel Lopez Alonso**

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**Convective instabilities in rotating fluids.**

Instabilities arising from the competition between convective heat transport and those forces due to rotation such as Coriolis or centrifugal buoyancy explain the onset of several large-scale atmospheric and astrophysical processes. The aim of our research line is to understand the complex dynamics derived from these instabilities. In order to do this, we approach numerically the Navier-Stokes equations for fluids confined in very simple domains. Direct numerical simulations, linear analysis of stability, continuation methods or dynamical systems theory are some of the mathematical tools used to carry out our studies. By mean of these techniques, we look for preturbulent flows and bifurcations occurring among them in order to explain the transition from a laminar basic flow to fully developed turbulence. A proper understanding of these flows would provide us essential information about phenomena such as cyclones formation or mass transfer in accretion disks.

*Keywords:* Convection, rotating fluids, numerical simulations

## Session II. Computational

chairman: Narcís Miguel

### 1. Andrés Aragonese Aguado

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#### **Distinguishing signatures of determinism and stochasticity in spiking complex systems**

The skipping activity of a semiconductor laser with optical feedback may look apparently random. I describe a method to infer signatures of determinism and stochasticity using ordinal time-series analysis. This method allows to classify experimental data in two categories that display statistically significant different features. One category is consistent with waiting times in a resting state until noise triggers an event, and the other is consistent with events occurring during the return to the resting state, which have a clear deterministic component. The method I describe can be a powerful tool for inferring signatures of determinism in the dynamics of complex systems in noisy environments, at an event-level description of their dynamics.

*Keywords:* time-series analysis, complex systems, semiconductor lasers, optical feedback, time delays

### 2. Elena Tamayo-Mas

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#### **Can maths help to predict degradation of materials?**

As soon as a structure is constructed, it starts to degrade. In order to understand this deterioration, laboratory experiments can be carried out. Nevertheless, there are several reasons (some laboratory investigations may be expensive or even dangerous...) why numerical simulations may be useful as a complementary method. Driven by this need and as a basis for these numerical simulations, theoretical models (e.g. damage or plasticity models) should be developed.

In this talk, damage models will be presented. Regarding numerical simulations, if these models are used, a strange phenomenon is observed: as the finite element mesh employed in the simulations is refined, the energy dissipated during the process tends to zero. Therefore, and in order to overcome this limitation, some special techniques should be incorporated into the model. In this work, different solutions to remedy this physically unrealistic behaviour will be explained.

*Keywords:* Numerical simulations, Finite Element Method (FEM), Material failure, Damage models, Regularisation

### 3. Igor Barahona Torres

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#### **The level of adoption of analytical tools in Barcelona, Spain**

The Level of Adoption of Analytical Tools (LAAT) on management is the extensive use of data, information technology and statistical methods in order to predict trends reduce risk and make more accurate decisions. For the purpose of measuring and quantifying the

degree of adoption of analytical tools at companies, a five level scale is proposed. This scale is a mixture of five key-drivers (KD's): Data-Based Competitive Advantage, Management Support on Data Analysis, Systematic Thinking and Communication Outside the company. The pattern is: the better at the key drivers, the higher at the scale a company is. At first, a questionnaire was designed and sent to 6,000 companies, all of them located on Barcelona Spain. We received 255 responses. Later, a set of seven statistical tools were integrated to extract relevant information from our dataset; among them, regression analysis, factorial analysis, correspondence analysis and logistic regression. This sequential integration of statistical methods, concepts, tools and information technology is a documented case of statistical engineering.

*Keywords:* -

#### 4. **Toni Vallès Català**

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##### **Identifying significant node groups in complex networks**

Complex networks enable an accurate representation of a large amount of information, with which a wide variety of problems can be solved. For instance, the spreading of a disease can be studied with the worldwide air transportation network, and metabolic networks provide methods to uncover novel drug targets within the every-increasing amount of biological data available. By studying the structure of a network we can extract all the information that can be used in the process of decision making.

A good approach is to identify the stochastic block models that capture the patterns of connections between nodes. However, a single stochastic block model might not suffice to capture all the different patterns of connection observable in the structure of a network, because connections between nodes might have arisen due to more than one independent mechanism. Our goal is to develop a method that identifies different stochastic block models, one for each mechanism responsible for the pattern of connection we observe.

We apply the method to a karate class network, which nodes are the class members and they are connected depending on their friendship. Due to a conflict among the class members the club split into two different academies, our method allows the identification of the two sides.

*Keywords:* Grouping Nodes, Stochastic Block Model

#### 5. **Sergey Kozlov**

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##### **Computational Chemistry for Nanostructuring Effects in Heterogeneous Catalysis**

The rapid growth of computational power in the last decades has made computational chemistry methods an important tool in present day chemical investigations. Today electronic structure calculations, such as those based on density functional theory, are able to provide deep qualitative insights in many chemical processes at such atomistic detail that would be hardly possible to obtain experimentally. However, the application of such methods to simulate heterogeneous catalysts with realistic nanoscale structure poses quite a challenge due to immense complexity of the latter, which requires employment of very big and computationally demanding models. In this contribution, a strategy to circumvent this

problem by employing well-thought moderately sized models is presented. The application of such a strategy is exemplified by a study of H adsorption and absorption into Pd and Pt nanoparticles supported on MgO, a process that may take place under typical catalytic conditions in a hydrogenation reaction. The results show that both nanostructuring of transition metal and the amount of H on the nanoparticle surface are important factors in hydrogen absorption.

*Keywords:* Heterogeneous Catalysis, Transition Metals, Nanoparticles, Hydrogen, Density Functional Theory

## 6. Arturo Valdivia

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### A Swiss knife for interdisciplinary studies

At first glance, one may not dare to point out equivalences between epidemics and rumour spreading, suspended pollen particles and stock market prices, river levels and Internet traffic, chemical reactions and decision making, fluid turbulence and electricity prices, photosynthesis and bankruptcy, filtering of noisy signals and insider trading... However, similarities arise when we model these phenomena in terms of a stochastic process, one of the main objects of study in theoretical and applied probability.

In this presentation we shall discuss examples of stochastic processes that may motivate interdisciplinary studies, linking different branches of experimental and social sciences.

*Keywords:* Interdisciplinarity; Probability; Stochastic processes

## 7. Hernán Pino Quintana

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### Calcular o simular?

Donat un sistema conformat per diversos elements amb interacció entre ells com podem predir la seva evolució? Aquest problema que en principi pot semblar específic i fàcilment soluble, amb les eines matemàtiques que avui dia disposem resulta molt difícil de resoldre analíticament. En aquest punt entra en joc el concepte de simulació en el qual, donat un sistema en el que tenim un gran control sobre els paràmetres que poden determinar la seva evolució, imitem el cas del nostre problema específic.

Utilitzant el mètode de simulació podem obtenir resultats amb mes rapidesa i precisió. Per abordar aquest camp es veuran les característiques que ha de tenir un simulador per ser d'utilitat y els motius que impulsen a la utilització de sistemes d'àtoms freds per aquest fi. Per últim es mostraran dos tipus de simuladors que han tingut un paper clau, basats en xarxes òptiques i camps *gauge* artificials amb les seves respectives aplicacions.

*Keywords:* simuladors quàntics, sistemes d'àtoms ultra-freds.

## 8. Abel Carreras Conill

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### Estudi teòric del rotor de mestranol

Els darrers avenços en la síntesi química han permès crear nous materials amb interessants propietats dinàmiques, com per exemple l'existència dins de l'estructura del sòlid de fragments amb un alt grau de llibertat rotacional que actuarien com a rotors moleculars que poden presentar correlació.

Es presenta l'estudi, des de un punt de vista teòric, del comportament dinàmic d'un material, recentment sintetitzat pel grup del Prof. Garcia-Garibay [1], que presenta en el seu interior una estructura de metanol amb fragments de fenilè que, en base a les evidències experimentals, podria comportar-se com a rotors moleculars.

L'estudi teòric s'ha dut a terme emprant el mètode Monte Carlo i dinàmica molecular.

[1] Rodríguez-Molina, B., Farfán, N., Romero, M., Méndez-Stivalet, J. M., Santillan, R., & Garcia-Garibay, M. A. *Journal of the American Chemical Society*, 133(19), 72807283 (2011)

*Keywords:* rotor molecular, dinàmica molecular, Monte Carlo

## 9. Oriol Lamiel Garcia

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### **How do nanoparticles look like?**

Scientific Interest in nanoparticles has grown in the last years because of their special properties, which are sometimes very different from the bulk materials. Nanoparticles are of special interest in catalysis and many other scientific fields. These differential properties which make these nanoparticles and small clusters so special are closely related with their structure. In this work we will comment different approaches to predict the structure of these small nanoparticles showing some examples of nanoparticles structures obtained for different materials.

*Keywords:* Nanoparticles, clusters, titanium carbide, titania

## 10. Marc Mulet Gas

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### **Computational Chemistry Applied to Endohedral Fullerenes**

Computational chemistry is a branch of chemistry that uses principles of computer science to assist in solving chemical problems. Quantum chemistry is incorporated by means of different algorithms into codes to calculate the structure and properties of molecules and solids. Different approximations are used both for static calculations and dynamic simulations. Computational studies are carried out to assist in understanding experimental data, to predict properties of new molecules and to explore reaction mechanisms. Our research is mainly based on endohedral metallofullerenes (EMFs). Fullerenes are closed carbon cages constituted by an even number of atoms. Soon after their discovery in 1985, it was reported the possibility to host a molecule in the hollow cavity. Endohedral Fullerenes have attracted wide attention due to their new properties and potential applications. The aim of our studies is, by using mainly density functional theory (DFT) methodologies, to understand the behavior in terms of stability of the EMFs, characterize new isomers, elucidate their electronic structures and the relation between them and the stability of different isomers. We also use these techniques in collaboration with experimental groups to support their research focused in the synthesis of new endohedral metallofullerenes and in the study of their formation mechanism.

*Keywords:* Computational Chemistry Endohedral Fullerene

## Session III. Material

chairman: José Manuel Rebled

### 1. Alberto Eljarrat Ascunce

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#### **Signal analysis methods applied to electron energy loss spectroscopy**

Electron energy loss spectroscopy (EELS) studies the energetic loss suffered by an electron beam when transmitted through a thin material sample. Nowadays, EELS can be performed as an everyday technique in the modern scanning transmission electron microscope (STEM), with energy and spatial resolutions below the eV and the nm. The analysis of EELS is divided in the two (overlapping) parts of the spectrum; the low-loss, that includes everything from 0 eV till the relative fading of the plasmon tail; and the core-loss, beyond this energies. Because of its versatility and increasing resolution, EELS has grown to be valuable technique in the arsenal for anyone interested in material analysis at the greatest possible resolution.

In this flash talk, the main tools for EELS analysis in the STEM will be addressed through examples extracted from real-life work. This work is mainly centered in the analysis of the low-loss part of the EELS, from semiconductor samples. So, the talk should cover all the properties that can be measured from a semiconductor sample in a low-loss EELS experiment at high resolution; band gap measurement, bulk plasmon analysis, and other valence band-related properties. Also, a brief report of works performed in core-loss EELS will complete the talk with the use of advanced tools like multivariate data analysis techniques.

*Keywords:* EELS, STEM, III-V compound semiconductor, MVA

### 2. Lluís Yedra Cardona

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#### **EEL spectroscopic tomography: 3D chemical information in nanomaterial analysis**

Electron tomography is a widely spread technique for recovering the three dimensional (3D) shape of nanostructured materials. Using a spectroscopic signal to achieve a reconstruction adds a fourth chemical dimension to the 3D structure. Up to date, energy filtering of the images in the transmission electron microscope (EFTEM) is the usual spectroscopic method even if most of the information in the spectrum is lost. Unlike EFTEM tomography, the use of electron energy-loss spectroscopy (EELS) spectrum-images (SI) for tomographic reconstruction retains all chemical information, and the possibilities of this new approach still remain to be fully exploited. In this work we prove the feasibility of EELS tomography at low voltages (80kV) and short acquisition times thanks to the recent advances in TEM and the use of Multivariate Analysis (MVA), applied to  $\text{Fe}_x\text{Co}_{(3-x)}\text{O}_4@ \text{Co}_3\text{O}_4$  mesoporous materials. This approach provides a new scope into materials: the recovery of full EELS signal in 3D. Data acquisition was carried out on a probe Cs corrected FEI Titan operated at 80 kV acceleration voltage. The whole data set consisted of 48 SI ranging from 68.99 to -64.74 following a Saxton scheme angle step with 55x55 spectra each, acquired during 0.1s.

High angle annular dark field (HAADF) signal was acquired simultaneously. Afterwards, for data treatment, MVA methods were applied, namely principal component analysis (PCA) and independent component analysis (ICA). From the noisy raw spectra, enhanced OK, Fe (L3,2) and Co (L3,2) edges were retrieved after PCA analysis. ICA successfully retrieved the Fe oxide and Co oxide signals of the sample as well as the background signal before the oxygen K edge (fig.1).

Reconstruction of those signals was achieved, leading to volumes not only containing structural information, but also chemical information (figure 2 a-f). Regarding chemical information, an interesting result was revealed: the comparison between iron and cobalt signals showed that some of the iron which was intended to penetrate into the structure remains instead on the outer surface (fig. 2h).

The particles are richer in iron at the border and therefore, iron related chemical signals give a sharp interface between the particle and the background, where HAADF signal is very low and has fallen to background levels due to the small thickness. These results show that iron signals reconstruct more precisely the edge of the particles than HAADF. On the other hand, the thickness signal has the drawback of underestimating the border more than the HAADF signal (fig. 2i). However, the most interesting feature of this signal is that it is insensitive to the chemistry of our sample and independent of multiple scattering, a characteristic not found in any other signal used for electron tomography. As a conclusion, EELS SI tomography is shown to be able to reconstruct chemical information of a sample in three dimensions. Moreover, the application of MVA to the data opens a new range of applications, reducing the limitations due to beam sensitive materials or samples with components with overlapping edges, where core-loss extraction using background estimation fails.

*Keywords:* TEM, EELS, tomography, nanomaterials

### 3. Victor Manuel Freire Soler

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#### **Synthesizing Graphene by Chemical Vapor Deposition**

This work is devoted to grow graphene on copper substrates by thermally activated chemical vapor deposition. Growing processes were performed in a quartz tube oven at a base pressure of 10<sup>-5</sup> Pa. The copper substrates consisted on two series of samples: A) monocrystalline copper (111) with an area of around 1 cm<sup>2</sup> and B) a pristine copper layer deposited on a polished c-Si wafer (100) by sputtering from a copper target (99.99% purity). A nickel diffusion barrier of 100 nm was used to avoid Cu diffusion into c Si. In both cases, the activated copper substrate was exposed to methane gas at 10<sup>-4</sup> Pa and annealed below 1000°C. The samples were characterized by scanning electron microscopy (SEM) and Raman spectroscopy. Raman analysis assessed the formation of graphene of one and two layers by showing the characteristic 2D band and the ratio 2D/G  $\geq$  1. In addition, SEM study provided evidences of layer by layer graphene growth.

*Keywords:* Graphene, CVD, monolayer, Raman, copper

### 4. Raquel Cumeras Olmeda

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#### **A Gas Sensor: the Ion Mobility Spectrometer**

Ion Mobility Spectrometry (IMS) is an analytical technique based on ion separation in gaseous phase due to the different ion mobility in an electric field. The IMS technology has fundamental advantages: high resolution ( $\sim$ ppb), fast measurements ( $\sim$ ms) and that ionization and characterization of the sample in IMS instruments occurs at ambient pressure [1]. Efforts for reducing size and cost while maintaining performances are being made by different groups [2-3], and the work presented here is part of such approach, using micro-technologies for its implementation. These advantages make IMS a rapidly advancing technique with a wide spectrum of applications, including detection of narcotics, CW agents and explosives [2].

Experimentally had been see that the mobility  $K$  ( $\text{cm}^2/\text{V}\cdot\text{s}$ ) of ions at constant temperature and pressure through a drift gas with density  $N$  ( $\text{m}^{-3}$ ), subject to an high electric field  $E$  ( $\text{V}/\text{cm}$ ) doesn't remain constant, and that its dependence with the field ( $E$ ) can be expressed as [4]:  $K(E/N) = K_0[1 + \alpha(E/N)]$ , where  $E/N$  is the normalized electric field and is expressed in Td (Townsend;  $1\text{Td}=10^{-17}\text{V}\cdot\text{cm}^2$ ) being  $K(E/N)$  the mobility of the ions and  $K_0$  the mobility coefficient under low or zero field;  $\alpha(E/N)$  is a function that takes account of the ion mobility dependence on electric field.  $K_0$  and  $\alpha$  are specific for each type of ion.

A first prototype of micro planar high field asymmetric IMS (p-FAIMS) has been fabricated in a sandwich-like configuration. It includes 3 different regions: 1) ionization region (where gas is ionized using a UV lamp); 2) filtering region (where the separation voltage VRF (V) and a compensation DC voltage VC (V) are applied in order to attract non desired ions to the plates while allowing the fly of the target vapour ions); 3) detection region (where desired ions are collected). The dimensions of the IMS chamber are: 20mm long, 5mm wide and 0.5 mm high (50  $\text{mm}^3$  in volume) and the pairs of electrodes are 1 mm each other.

p-FAIMS has been analyzed for two risky-healthy volatile organic compounds: 2-propanone and toluene. Gas sensing test of the sensors was carried out in a continuous flow. 2-propanone was generated in a bubbler with a flow of nitrogen of 1.6 L/min leading to a concentration of 1000 ppm. While toluene was generated using three mass flow controllers (Brooks 5850E), and mixtures of nitrogen (Praxair) and the analyte (Toluene, 200 ppm) were adjusted in order to obtain the desired concentration. The ionization electrodes were biased to 0 V.

For the study of 2-propanone, in the filtering electrodes, the RF voltage amplitude was varied equitably over all the filtering electrodes, being varied from 0 V to 350 V for a frequency of 2 MHz, and the compensation voltage was scanned from -5 V to +5 V with a step of 0.5 V. The voltage applied to the detector electrodes was -4 V. Detection of 2-propanone is shown in Figure 2 for a CV scan. The intensity detected is about 22 pA and the CV for 2-propanone is +0.5 V.

In the study of toluene, also the reverse flow conditions study was carried out. No filtering conditions were done for the first step, and detection was done in the filtering region for a voltage of -5V. In Figure 3 is shown the result as function of reverse total flow for a constant toluene flow of 50sccm. Maximum intensity is obtained for a total flow of 150sccm.

These results demonstrate the viability of operation of this new p-FAIMS, being reduced the encapsulation system, and the cost in device manufacture.

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*Keywords:* VOC, p-FAIMS, Ion Mobility Spectrometry, Gas Sensor

## 5. Abel Fontserè Recuenco

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### High Power Electronics HEMT GaN based Devices

Power Electronics plays a key role in the generation-storage-distribution cycle of the electric energy. This is because the main portion of the generated electric energy is consumed after undergoing several transformations, many of them carried out by power electronic converters. Examples of this can be found in all ranges of power levels (from a few W to MW), and they include many types of different equipment (power supplies for computers, industrial and telecom systems, domestic appliances, motor drives, industrial converters, etc.). The largest portion of the power losses in these power electronic converters are dissipated in their power semiconductor devices.

Nowadays, these devices are based on the mature and very well established silicon technology. However, silicon exhibits some important limitations regarding its voltage blocking capability, operation temperature and switching frequency. Therefore, a new generation of power devices must be developed for power converters in applications where converters based on traditional silicon power devices cannot operate. The use of these new power semiconductor devices will allow increasing the efficiency of the electric energy transformations achieving a more rational use of the electric energy.

Novel and innovative power devices based on Wide Band Gap (WBG) semiconductors can play a main role in energy efficient systems. Among the possible candidates to be the base materials for these new power devices, SiC and GaN present the better trade-off between theoretical characteristics (high-voltage blocking capability, high-temperature operation and high switching frequencies) and real commercial availability of the starting material (wafers) and maturity of their technological processes.

*Keywords:* Power Electronics, HEMT, GaN, AlGaIn/GaN, 2DEG

## 6. Stefanos Chaitoglou

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### Arc-Discharge Synthesis of Fe@C Nano particles for General Applications

In the present work we investigated in the synthesis and characterization of core@shell nanoparticles. The reactor works in Arc-Discharge and spherical iron nanoparticles coated with a shell of carbon were obtained at near-atmospheric pressure conditions ( $58 \times 10^4$  Pa).

The current was always 40  $\alpha$  and the the studied concentration range of the Fe into isoocane varies between 1% w/w and 4%w/w. Also the studied flow of the precursor gas varied from 30ml/min to 120ml/min. The resulting diameter of the iron core is between 5-9nm as we could measure by transmission electron microscopy (TEM). From the selected area electron diffraction (SAED), the nanoparticles appear to have a crystalline dense iron core. From the energy-dispersive X-ray analysis (STEM-EDX) we have verified the absence of oxygen in the core. The magnetic properties of the nanoparticles have been investigated up to 5K temperature using a superconducting quantum interference device (SQUID). The results reveal a superparamagnetic behaviour, narrow size distribution and an average diameter of 6 nm of the nanoparticles having a blocking temperature near 40 K.

*Keywords:* Nanomaterials, Fe@C Nanoparticles, Arc-Discharge, Superparamagnetism

## 7. Víctor López Domínguez

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### **Colossal Reduction in Curie Temperature Due to Finite-Size Effects in Nanoparticles**

In this flash talk, I show the enormous effect on the ordering transition temperature, in ultrasmall CoFe<sub>2</sub>O<sub>4</sub> nanoparticles. The lattice distortion in the inverse spinel structure affects the exchange interaction between the different atoms, reducing the Curie temperature 100 times. The experimental and theoretical results are an unreported magnetic behavior in nanomagnetism, suggesting its further study as an advanced material.

*Keywords:* Magnetic nanoparticles, Curie Temperature, nanotechnology

## 8. Carlos Heras Paniagua

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### **Synthesis and study of new organic molecules that show magnetic properties**

The aim of this work has been the synthesis of new molecules, apparently closed shell, but they are in a biradical state. The construction of the theoretical model is based on the wave function ab initio of the functionals RHF, UHF, ROHF and CASSCF to construct potential energy surfaces corresponding to the singlet closed shell and triplet electronic states. The reaction path connecting the two minima singlet-triplet passes through a point of intersection. The reaction coordinate of this path is mostly concentrated in the dihedral angle that characterizes coplanarity between the two aromatic rings of the molecule bound by a unit of the type C-N=O;O;C.

Thus, it's reached thermally a conformation associated with triplet electronic state that is different from planar singlet closed shell, which is responsible of observed paramagnetic character. Finally, we made O;O;measurements of the magnetic nature of the organic material. The results are consistent with studies on the origin of magnetism in these molecular species and has enabled us to understand the basis.

*Keywords:* organic material, magnetism, theoretical study

## 9. Estefanía Lopez Marne

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### **An Experimental and Theoretical point of view of ion-molecule reactions**

Collisions between ions and neutral molecules are very important in scientific studies, and we can find them in the study of atmospheric processes, gas-phase catalysis or different types of plasmas. In the last years GQRD group study has been focused in excitation and charge transfer processes in several systems composed of alkaline ions and neutral molecules. To carry out the reactions our group use crossed molecular beams techniques, and studies the different fragments formed in the collision by a quadrupolar mass analyser.

*Keywords:* ion-molecule reactions, dynamics

#### **10. Claudia Trejo Soto**

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##### **Fluid Interfaces in Microchannels**

We study the interface fluid-air of water and other viscous fluids such as ethylenglycol inside microchannels of different height and width. The fluid-air interface moves by the action of a constant pressure exerted by a liquid column submitted to atmospheric pressure. We fixed different heights and measured the velocity at which the interface of fluid is moving at different positions of the microchannel. By using Darcys Law we obtain a relation with the fluids viscosities. We have observed that for heights over the 2.5 cm the velocity of the remains constant. We have performed measurements with blood at 45% of hematocrit.

*Keywords:* Interface, Darcy Law, Viscosity

#### **11. Jordi Prat-Camps**

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##### **Shaping static magnetic fields**

Magnetic fields are widely used in science and technology to generate power, store information, perform medical tests, etc. Our work explores novel ways of controlling magnetic fields, allowing to avoid and/or overcome some classical limitations. Applying the transformation optics technique to the case of static magnetic fields we have made realistic proposals to cloak a region from magnetic fields or to transport magnetic energy from a source to a distant point through the free space.

*Keywords:* magnetism, cloaking, transformation optics, metamaterials

#### **12. M. Carmen Miguel López**

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##### **Mechanical deformation of curved crystalline shells**

Crystals must deform to fit on curved surfaces. The energy cost associated to such deformations consists of both stretching and bending contributions. According to Euler's theorem and the Euler characteristic of the surface, the minimum energy configuration contains geometrically necessary topological defects, all of which share an elementary building block: the disclination. The elastic cost of a disclination in a crystalline membrane is very high, but buckling and/or the proliferation of boundary scars can reduce it considerably. We will briefly discuss the structural transitions and the microstructure dynamics undergoing the continuous mechanical deformation of curved crystalline shells as a function of

effective bending rigidity, sample size, and geometry. The quasi-static deformation of these structures is characterized by intermittent dynamics with collective particle reorganizations mediated by the proliferation and dynamic delocalization of defects. At large deformations we eventually observe failure phenomena such as the melting or the cavitation of the crystal shells.

*Keywords:* deformation, microstructure, curvature, defects, failure

### 13. Marina Mariano Juste

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#### **Efficient fabrication of organic solar cells by the dip-coating method**

Organic solar cells have been the subject of research for the realization of portable, flexible and transparent modules as renewable energy sources. We investigate the deposition of the active layer of such type of devices using a very simple and cost effective fabrication method based on the dip coating procedure. We demonstrate that this procedure can be used for fabricating bilayer, as well as bulk heterojunction solar cells. We fabricate polymeric cells using poly(3-hexylthiophene) (P3HT) as donor layer and phenyl-C61-butyl acid methyl ester (PCBM) as acceptor. There is no difference in cell performance between the ones fabricated by dip coating and the more traditional spin coating. Additionally, we observed that the coating solution can be used many times to fabricate cells in a continuous mode with a small dispersion of only 8% on the photovoltaic behavior. The dip-coating technique opens an alternative route for a cost effective large scale production of high efficiency organic solar cells as the spray coating or the inkjet printing.

*Keywords:* organic solar cells, dip coating, air processed OPV

### 14. Anna May

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#### **Synthesis of functionalized nanoparticles for the control of internal hemorrhage**

In this flash talk I would like to talk about the project that I've been doing at UCSB about the synthesis and functionalization of silica nanoparticles for the control of internal hemorrhage.

Metal oxides, zeolites and clays have been studied for the past years for the control of external hemorrhage. The idea is to use these materials also for internal hemorrhage. However, internal injuries pose a great challenge due to inaccessibility, so treatment strategies must consider particle size, concentration thresholds, selectivity and biocompatibility. Issues that are not that important for external wounds but crucial for internal ones.

We have been synthesizing silica nanoparticles, known to be procoagulant agents, and we have functionalized them with polyphosphate. Polyphosphate is produced by human platelets during the coagulation process and their procoagulant properties have also been described. Moreover, we have engineered the protection of the particles for prolonged exposure in the body while also targeted to activate only at the wound site.

*Keywords:* Internal hemorrhage, silica nanoparticles, functionalization; in general: materials, biochemistry.

## Session IV. Environment

chairman: Albert Bruix

### 1. Albert Ossó

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#### **The Mystery of recent stratospheric temperature trends**

A new dataset of middle and upper stratospheric temperatures based on reprocessing of existing satellite radiances provides a strikingly different view of the recent stratospheric climate change than that provided by existing datasets. The new data call into question our understanding of observed temperature in the stratosphere and the processes that determine its evolution. Here we highlight those differences and offer suggestions for how the climate community can resolve this mystery.

*Keywords:* Stratosphere, Temperature, Climate Change

### 2. Jagos Radovic

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#### **Tracking the Deepwater Horizon oil spill**

On April 20, 2010, the exploratory ocean drilling rig Deepwater Horizon exploded releasing an estimated 4.9 million barrels into the Gulf of Mexico, making it the largest oil spill in U.S. history. More than two years after the spill, oiled samples still can be found along the Gulf beaches containing refractory organic molecules that provide invaluable clues for the sample identification (fingerprinting). This presentation will show the application of comprehensive two-dimensional gas chromatography (GCxGC) for the characterization of oil impacted samples to track the fate of oil in the marine environment.

*Keywords:* Gulf of Mexico, oil spill, biomarkers, fingerprinting, comprehensive two-dimensional gas chromatography (GCxGC)

### 3. Jordi Baró i Urbea

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#### **Earthquakes inside a thimble-sized porous glass**

It is long known that, instead of being random events, earthquakes happen as a consequence of the jerky dynamics taking place when Earth's crust is driven by plate tectonics. The microscopic description of the process needs to be understood as a complex systems where non-trivial long range interactions can give rise to a scale-free endogenous production of seismological activity.

In our recent experiment, we recorded acoustic signals during the mechanical failure under compression of a porous material, and we found the fulfillment of some statistical laws well studied for earthquakes. Among them stands out the unified scaling law for recurrence times. This common behavior can be a trace of a hidden Universality class that may help to characterize both brittle fracture of materials and seismological activity.

ref: <http://arxiv.org/abs/1211.1360>

*Keywords:* extreme events, complex systems, material science, geophysics, condensed matter

4. **Aitor Rumín Caparrós, Oriol Veres Cucurella, Rut Pedrosa Pàmies**

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**Marine sedimentary particles as drivers of the deep marine ecosystem**

Deep-sea marine ecosystems spread across about 60% of the Earth's surface so that altogether they constitute the most extensive cluster in the world. The functioning of these ecosystems relies on the interrelations and interdependences in between the geological setting (sediment sources and its characteristics), physical processes (meteorological conditions and hydrodynamic characteristics of the water masses) and biogeochemical aspect (origin, evolution and nutritional value of the organic matter).

The integrated study of these components allows understanding in which way and to what extent the external atmospheric signal is transmitted towards the deep sea, thus controlling the dynamics of particle fluxes along continental margins and subsequently the community structure and the population dynamics of its living organisms. Particle fluxes in the water column can be measured by deploying mooring lines equipped with automated sediment traps, current meters and other instruments. Once collected, settling particles have to be analyzed to obtain the total mass flux, the main constituents' composition (lithogenic fraction, calcium carbonate, opal and organic matter), grain size distribution and many other parameters after sets of analyses.

These data allow us to better understand the interactions in the continuum atmosphere-water column-deep-sea floor. These studies have important implications for quantifying and modeling the global carbon cycle, which is intimately linked to the on-going global warming through CO<sub>2</sub>.

*Keywords:* Deep-sea marine ecosystems, marine geology, biogeochemical fluxes

5. **Daniel Seco**

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**Mathematical analysis for the antarctic ice**

Recently I discovered the three topics I deal with in my Thesis are connected by one application: the shape and size of the ice layer over glacial oceans. The techniques and theory developed to study this phenomenon involves studying fractal properties of large scale ice structures, sharp signal processing and spectral analysis of the interior composition of ice blocks.

*Keywords:* fractals, sampling, zeros of complex polynomials

6. **Elena Galán del Castillo**

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**Sustainable farm systems and transitions in agricultural metabolism: the end of traditional organic agricultures in Mediterranean Spain**

Our agricultural systems nowadays rely on the consumption of fossil fuels. In a peak oil scenario (with oil prizes rising up) the fossil way will be forced to be left towards an agriculture more based on organic energy sources. Was there a time in history when the two systems co-existed? Was there a time in history we had the chance to choose between organic and fossil? The First Globalization (1870-1930) triggered a market-driven race for yield increases in the prevailing organic agricultures of the Mediterranean Spain, which ran

into several agro-ecological limits up to the point when further increases were not possible without degrading at the same time the biophysical structures of agro-ecosystems. Was there room for the existing organic agricultures to increase further their yields without taking the path of the Green Revolution? Had they really exhausted all their organic capabilities? We reconstruct the cropland nutrient balances and the energy flows of the agro-ecosystems in order to analyze the transition of the organic agricultures in Catalunya during the period 1870-1970.

*Keywords:* energy balance, nutrient balance, Mediterranean agriculture, organic agriculture, agricultural metabolism

## 7. Mercè Bermejo Cisneros and Patricia Povea de Castro

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### **Past climate changes: from millions to tens of years**

The oceans play a crucial role in the global climate system through the thermohaline circulation and also absorb one third of emissions from the use of fossil fuels and tropical deforestation. Paleoceanography is the study of past climate by analyzing records as marine sediments and is therefore an excellent tool to increase the understanding about the mechanisms that modulate climate change. The analysis of these sediments, both lithic and the biogenic fraction in different parts of the world, give important information about the transport processes that have taken place at the bottom of the ocean and also about weather conditions at that time. Regarding that biogenic fraction characterizes both surface (planktonic foraminifera) and deep water (benthic foraminifera). The study of these fractions allows to obtain information of great importance when it comes to reconstructing past climate changes, both in recent millennia (Site HER-MC-MR3) and for periods of 2 million years ago (Site ODP 1240). To reconstruct past oceanographic changes there have been several indicators analyzed: grain size composition, stable isotopes (C and O) and ratio Mg / Ca measured in planktonic foraminifera *Globigerina bulloides* and benthic species *Uvigerina* sp. The results are also compared with data obtained from elemental composition of the sediment with X-ray fluorescence scanner. In addition, analyzes for Total Organic Carbon (TOC) have been performed. These parameters allow the reconstruction of water temperature, deep currents intensity, atmospheric circulation changes and many oceanographic and climatic variables.

Site HER-MC-MR3 was retrieved north of the island of Minorca, to obtain characteristics of the Northwestern Mediterranean climate of the recent millennia (latest Holocene), which could also help to distinguish between the natural and the anthropic change factors. Moreover, ODP 1240 record gives us information about the atmosphere-ocean teleconnections during the Pleistocene (1.6 to 2.25 Ma) controlled by migrations of the Intertropical Convergence Zone (ITCZ) during this period.

*Keywords:* Paleoceanography; climate change; Mediterranean sea; Pacific Ocean; Surface and deep water; Planktonic and benthic foraminifera

## Session V. Biology

chairwoman: Anna Alemany

### 1. Esther Ibáñez Marcelo

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#### **Evolutionary dynamics of populations with genotype-phenotype map**

There is a complex relationship between genotype and phenotype. One of the outstanding features of this map is that is not a one-to-one map, because many genotypes are compatible with the same phenotype. Whereas genes are the entities passed on from one generation to the next and their frequencies measured over populations (the remit of population genetics), selection acts at the level of phenotypes. Thus, assigning fitness values to genes (mutant variants, different alleles, etc.) is not, in general, the valid approach. We are trying to put forward some of new properties we may expect to emerge when the genotype-phenotype difference is taken into account, both in a general setting and in particular cases related to disease. We have been focused on formulating models of evolutionary dynamical processes with genotype-phenotype map, give a definition of phenotype based on the attractors of simple models of the dynamics gene regulatory networks, and simulate it in order to ascertain its dynamical properties. We have introduced a bipartite network to study genotype and phenotype together and their structural relationship. Also a way to understand their structure is to study their clustering coefficient, existence of communities, which are related to phenotypic robustness, or connectivity between communities (it means, innovation).

*Keywords:* genotype-phenotype, complexity, genetic network, dynamics, robustness, innovation

### 2. Daniel Sánchez Taltavull

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#### **Optimal transition paths of stochastic cell differentiation systems**

Tissues in higher organisms exhibit a hierarchical structure where only a small number of stem cells have the potential for indefinite division. The descendants of the stem cell population undergo a process of maturation where, after a series of intermediate differentiation steps, a fully matured cellular type emerges. In general, mature cells have no replicative potential whereas cells belonging to the intermediate stages gradually lose their stem cell-like properties. Acquiring a proper understanding of this process is important for many reasons but one of the more pressing issues is related to the fact that dysregulation of the maturation process leads to cancer. However, many questions related to the regulation of this process remain unclear. Our aim is to examine some of these open questions. Specifically, it has been suggested that the number of differentiation stages between self-renewing stem cells and fully-differentiated cells plays a major role in the evolutionary stability of cell populations. We will formulate a stochastic model of stem cell maturation with resource limitation to account for homeostatic constraints. Here we examine how the introduction of symmetric stem cell division affects the stability of the whole population and extinction times studying the transition paths between the metastable states that appear for the symmetric division.

*Keywords:* Cell population, Stem cells, population dynamics, Stochastic chemical kinetic systems, Stochastic processes, Transition paths and transition rates.

### 3. Laura Gonzalez Claramonte

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#### **Quartz Tuning Fork based nanosensors for biological Scanning probe microscopy**

Quartz tuning fork-based sensors are self-sensing probes and their use is growing in Scanning probe microscopy. They do not need a laser-photodiode system and they have a higher quality factor in liquid than standard cantilevers. Nevertheless, a few studies on soft biological samples have been reported using these probes. One of the main limitations of tuning fork probes is that they are usually handmade because there are no commercial probes suitable for a wide range of experiments are available. The working principle, fabrication and experimental results in the nanocharacterization of different samples are presented by using different working modes.

*Keywords:* self-sensing probe, atomic force microscopy, quartz tuning fork

#### **4. Juan Camilo Luna**

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##### **Mathematical modeling of regulatory processes during development**

Development is a process in which, from a homogeneous state comprising a small group of identical cells, an entire organism with several different cell types is formed. Development involves pattern formation since cell types organize in different shapes forming heterogeneous states. The temporal and spatial determination of cell fates depends on the regulation of the transcriptional activity, which involves genetic expression and signaling processing. The mechanisms underlying the regulation of genetic expression are of great importance in regard to the final pattern observed in tissues and organs (which in terms of development is an output). Although different mechanisms of regulation are able to explain the same output, they can also imply very different behaviors once the conditions have changed. Modeling of dynamic regulation process during development provides a powerful tool in order to discern which mechanisms are more likely to explain the outputs observed. We introduce briefly an example of this situation in a study of pattern formation during the development of the inner ear of the chick.

*Keywords:* modeling, developmental biology, pattern formation

#### **5. Tomás Luque González**

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##### **Local micromechanical properties of decellularized lung scaffolds measured with atomic force microscopy**

Bioartificial lungs reengineered from decellularized organ scaffolds are a promising alternative to lung transplantation. Critical features for improving scaffold repopulation depend on the mechanical properties of cell microenvironment. However, the mechanics of the lung extracellular matrix (ECM) is poorly defined. We measured local mechanical properties of the ECM in different regions of decellularized rat lung scaffolds with atomic force microscopy. Lungs excised from rats ( $n = 11$ ) were decellularized with sodium dodecyl sulfate (SDS) and cut into  $\sim 7 \mu\text{m}$  thick slices. The complex elastic modulus ( $G^*$ ) of lung ECM was measured over a frequency band ranging from 0.1 to 11.45 Hz. Measurements were taken in alveolar wall segments, alveolar wall junctions and pleural regions. The storage modulus ( $G'$ , real part of  $G^*$ ) of alveolar ECM was  $\sim 6$  kPa showing small changes between wall segments and junctions. Pleural regions were 3-fold stiffer than alveolar walls.

$G'$  of alveolar walls and pleura increased with frequency as a weak power law with exponent 0.05. Loss modulus ( $G''$ , imaginary part of  $G^*$ ) was 10-fold lower and showed a frequency dependence similar to that of  $G'$  at low frequencies (0.1–1 Hz) but increased more markedly at higher frequencies. Local differences in mechanical properties and topology of the parenchymal site could be relevant mechanical cues for regulating the spatial distribution, differentiation and function of lung cells.

*Keywords:* Biological scaffolds, extracellular matrix mechanics, alveolar mechanics, atomic force microscopy, bioengineered lungs.

## 6. Pau Formosa-Jordan

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### **Feedbacks, competition and cellular patterning**

Cell-to-cell communication through biochemical signals drives feedbacks of different types within and among cells. Often, these feedbacks are present in developing tissues, where cells initially equivalent become ultimately distinct, creating spatial patterns of different cell types. In this talk it will be shown from a theoretical scope how competition between different signaling elements can reshape feedbacks, driving unexpected behaviors and facilitating patterning. In particular, we will focus on how competition enables patterning of sensory cells in the vertebrate inner ear.

*Keywords:* Nonlinear dynamics, systems biology, cell signaling, pattern formation

## 7. Susana Perez-Alvarez

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### **Understanding HIV diversity: impact on vaccine development and treatment options**

HIV infection and AIDS affects millions of people around the world and there are still many questions to resolve. The difficulty responding to questions lies largely to the diversity of the virus itself, but also the diversity of the infected host.

We would like to present at JIPI the first steps of a PhD project that aims to study the diversity of HIV to support the main lines of current research - the development of a therapeutic or prophylactic vaccine, and treatment personalization in order to maximize its effectiveness - with the intention of progress in the cure or in the eradication of HIV. To achieve this, we propose the development of new tools that integrate Biostatistics and Bioinformatics knowledge.

This is a specially multidisciplinary project, integrating many sciences: statistics, computer science, immunology, medicine, ... In addition, this project links different research institutions: it is developed in one of the best research centers for HIV in Europe, the Irsi-Caixa Institute for AIDS Research from Badalona; and in collaboration with the GRASS research group from the UPC; and within the Catalan AIDS vaccine research project, the HIVACAT program.

*Keywords:* Statistics, HIV, medicine, biostatistics.

## 8. David Palau-Ortín

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### **Dynamics and stability of cellular decision making driven by biochemical signals**

Biology poses many examples of processes that can be understood in terms of bifurcations of nonlinear dynamical systems. Cells change of state according to biochemical signals in processes which are known as cellular decision making. Three ingredients are commonly associated to cellular decisions: multistability, biochemical signals and stochasticity. The dynamics underlying genetic interactions are typically nonlinear, and the nonlinearities are crucial to generate the multistability required to describe the multiple stable states involved in the differentiation processes. Stochasticity in cellular decision making arises partially from the inherent stochasticity of the genetic dynamics involved due to the low copy number of reactants.

In some cases cell differentiation takes place cell-autonomously, without cell-to-cell communication. In contrast, some other cellular decisions occur with cell-to-cell communication, creating an ordered spatio-temporal pattern of different cell types. Herein, we will present our theoretical studies on how these cellular decisions depend on the biochemical signals driving them.

*Keywords:* cell signaling, genetic circuits, pattern formation, cell differentiation

### **9. David Frigola Tubert**

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#### **Stochasticity, cell state switching and gene network architecture.**

Genetic networks are dynamic biochemical systems which frequently involve low copy numbers of reactants, making them inherently stochastic. This stochasticity has been known to affect their behaviour, either in benefit or in detriment. For instance, when these systems are bistable, fluctuations can enable stochastic switching from one cellular state to another. This switching can enhance the fitness of populations of unicellular organisms by allowing a variety of responses to uncertain environments.

Stochasticity of different origins and natures begets differences in the behaviour of this switching. For instance, we have seen theoretically that intrinsic (state-dependent) fluctuations drive asymmetric switching, which is consistent with experimental data previously reported.

Furthermore, stochasticity affects differently network topologies that would otherwise be equivalent. Recent results by others have shown that a possible reason for some network topologies to be chosen over others in biological evolution is their stochastic behaviour. I will talk about this interplay between genetic network topology and stochasticity of different origins.

*Keywords:* Genetic circuits, Stochastic switching, Intrinsic noise

### **10. Xavier Just Baringo**

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#### **Síntesi total d'antibiotics d'origen marí.**

Al llarg de les últimes dècades la preocupació creixent per la resistència als antibiòtics ha motivat un gran interès pel descobriment de noves substàncies que permetin combatre

aquesta amenaça. L'abundància d'espècies encara desconegudes que habiten a les profunditats de l'oceà són una font molt valuosa de noves entitats químiques que poden donar resposta a aquest reconegut problema de salut. Mitjançant la síntesi química podem validar l'estructura de compostos naturals que presenten l'activitat desitjada i aprendre els detalls del seu mecanisme d'acció. Al nostre grup de recerca ens hem centrat en la síntesi de dos compostos macrocíclics amb un perfil prometedor: l'aeruginazol A i la baringolina.

*Keywords:* antibiòtics, síntesi orgànica, productes naturals, tiazol, compostos macrocíclics

#### 11. **Laura Orellana**

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##### **Revealing cancer mechanisms by simulations - a bridge between physics and medicine**

We will explain in simple words a highly interdisciplinary project that combines physics, biochemistry and medicine. The epidermal growth factor receptor (EGFR) is the prototype of tyrosine kinase receptors, which regulate key functions in cells. In the presence of growth signals, the extracellular domain undergoes a dramatic change in shape from a closed inactive state to an open configuration, triggering cell division. Cancer-related mutations appear clustered in critical parts of this structure. We explored the motions of EGFR using a combination of coarse-grained and atomistic simulations, and we found that the molecule has intrinsic opening/closing movements that can be perturbed by some mutations targeting these regions, which act as hinges. Simulation of an aggressive mutation in one of the dynamical hot spots revealed a previously unknown active state, which is the hallmark of many tumors but has eluded so far experimental characterization. Based on the knowledge gained, we propose a novel model for EGFR activation that explains a number of experimental data and will help to develop better treatments for cancer.

*Keywords:* cancer mutations, protein structure, molecular dynamics, hinge

#### 12. **Maria Martí Pietro**

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##### **Single-molecule methods in biophysics**

Single-molecule techniques (like fluorescence, optical and magnetic tweezers or atomic force microscopy) allow to observe a single molecule at real time and at nanometric resolution. In the particular case of optical tweezers, mechanical forces of the order of tens of piconewtons can be applied and the behavior of the molecule under stress can be studied. Such methodologies pave the way of molecular biophysicists to study the folding problem of proteins and nucleic acids, the processivity of molecular motors under different conditions, or the binding interactions between a single pair of ligands and receptors, among others. In this talk, I will give a flavor of which are the experimental results and what it is done in this field.

*Keywords:* statistical physics, folding problem, molecular motors, acid nucleics, molecular interactions, optical tweezers

#### 13. **Joan Atcher**

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### **The emergence of halophilic evolutionary patterns from a dynamic combinatorial library of macrocyclic pseudopeptides**

A bio-inspired dynamic combinatorial library of macrocyclic pseudopeptides provides a simple model of environmental adaptation. The increase of the ionic strength amplifies the species bearing acidic side chains (anionic at physiological pH). This behavior has a close resemblance with the evolution observed for the proteins of halophilic microorganisms, which have adapted their biomolecular machinery to survive in hypersaline media, such as salt lakes.

*Keywords:* organic chemistry, supramolecular chemistry, dynamic combinatorial chemistry, systems chemistry, macrocyclic pseudopeptides, thiol-disulfide exchange

## **Session VI. Social phenomena**

chairman: Rubén Pérez

### **1. Michele Starnini**

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#### **Modeling human dynamics of face-to-face interaction networks**

Face-to-face interaction networks describe social interactions in human gatherings, and are the substrate for processes such as epidemic spreading and gossip propagation. The bursty nature of human behavior characterizes many aspects of empirical data, such as the distribution of conversation lengths, of conversations per person, or of inter-conversation times. Despite several recent attempts, a general theoretical understanding of the global picture emerging from data is still lacking. Here we present a simple model that reproduces quantitatively most of the relevant features of empirical face-to-face interaction networks. The model describes agents which perform a random walk in a two dimensional space and are characterized by an attractiveness whose effect is to slow down the motion of people around them. The proposed framework sheds light on the dynamics of human interactions and can improve the modeling of dynamical processes taking place on the ensuing dynamical social networks.

*Keywords:* Dynamical Networks, Social interactions, Human behavior, Modeling.

### **2. Juan Alvarez de Lara Cabrera**

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#### **Crowdfunding, new option for funding**

Facing the new economic situation that are affecting the funding for new projects, it appears new options to help these projects to go forward, develop and become businesses (tech, science, healthcare, and other fields). We will explain which is crowdfunding, how it works, advantages.

*Keywords:* crowdfunding, seedandclick, funding, entrepreneur

### **3. Pol Colomer**

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## Complex Networks

Most social, biological, and technological networks display substantial non-trivial topological features, with patterns of connection between their elements that are neither purely regular nor purely random. The study of these complex structures and the dynamics that take place on top of them is what is called network science. Ideas from network science have been applied to the analysis of metabolic and genetic regulatory networks, the design of robust and scalable communication networks, the development of vaccination strategies for the control of disease, the design of a marketing strategies and a broad range of other practical issues.

*Keywords:* Xarxes, Complexitat, social, Networks, Complex, epidemics

### 4. David Mateo Valderrama

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#### Research in search to search in research

Graph theory has induced a paradigm shift in the way we look at complex systems and our ability to study them. Densely interconnected graphs, such as social relations in most human activity, are now routinely explored and studied; not only for the insight in the fundamental working of these systems, but also for a practical understanding of our social world. This understanding leads to optimized and scalable information sharing and knowledge acquiring processes.

With this spirit on practicality, I present here my work on the design of algorithms to study a network of scientists connected through their collaborations in scientific literature. The aim for this is to develop a tool capable of detecting similar or complementary investigations and scientists that can benefit from one another, a tool that may even suggest potential interdisciplinary collaborations and help novel researchers keep track of what is done in their field more efficiently.

*Keywords:* networks, graphs, research

### 5. Antonia Godoy Lorite

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#### Long-Term Evolution of Email Communication Networks

he study of data from technological platforms as email, mobile or public transportation networks, can provide us with a better understanding of human communication patterns and hold the possibility to predict the future changes the network may undergo. In this work we focus on the long-term evolution of the anonymous email network provided by Rovira I Virgili University. Our findings show that, behind the aparent arbitrariness, the annual changes in communication growth between pairs of users resemble those featured in other human activities such as growth of companies or air transportation networks (M. Stanley et al., Nature 379, 804 (1996), A. Gautreau et al., PNAS 22, 8847 (2009)).

We show that the emails' growth between users of the network is exponentially distributed. We checked that the shape of the growth distribution between a couple depends on the amount of emails exchanged in the past. Even of greater importance is that distributions are not symmetric with respect to the center. This means that the processes governing the increase or decrease of the communication follow different mechanisms. Finally, we observe that the growths of different pairs are not independent.

The correlations patterns we found in the system will be used to build a model in order to predict evolution dynamics in arbitrary email networks. Development of such a work could be of great interest in the desing of secure and solid network of email servers.

*Keywords:* -

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### **Global Thoughts vs. Local Actions: Financial Markets Study Case.**

Nowadays we have huge amount of quantitative information that can be useful to study how humans behave. Many tools and models borrowed from Statistical Physics are more and more applied to describe this socio-economic context in a more scientific way. An specific case of a global variable (volatility) influencing the individual activity of investors is studied here. Such feedback mechanism, which can also be found in other fields (biology, sociology, game theory, etc), leads to the question about how important is the heterogeneity among the agents of their time horizon.

*Keywords:* Decision making, Financial markets, Time series analysis

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### **Embracing the world: Our brain combines optimally information from the different sensory modalities**

Perceiving consists in extracting from the environmental noise, that particular information which could become relevant for us (e.g. an incoming thread, a delicious piece of food). Classically in neuroscience, it is well known that visual system is specialized in deconstructing images from light, whilst the auditory system decompose changes in mechanical pressure to generate meaningful sounds. However, in ecological conditions, an apple is not only a taste, a color, a smell or a texture; it is better the combination of all of them, and our brain knows how to resolve these (multi)-sensory correspondences very well, making that even the particular visual information which represents the color, may easily affect our perception of its particular apple smell or taste. Thus, against the classical sensory-modular perspective, research in human and animal behaviour has shown how in perceptive processes, all the sensory systems are not so neuro-anatomically segregated as previously was thought, and instead exchange and combine information continuously in an optimal (bayesian) way to create a more precise and accurate representation of our external world. I will briefly present some experimental evidences of this multisensory interplay and what techniques are often applied for research in modern neuroscience.

*Keywords:* neuroscience, psychophysics, multisensory integration