6th Scientific Meeting of BCN-b PhD Students



Book of Abstracts

November 25-26,2021
UAB Campus

ICMAB
ICN2 Institut Català de Nanociència i Nanotecnologia
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PROGRAMME

Thursday 25th of November 2021		
Welcome Session		
Plenary Talk	**Prof. Xavier Obradors** Institut de Ciència de Materials de Barcelona (ICMAB CSIC)	**Clean energy transition: what can we expect from superconductivity?**
Plenary Talk	**Dr. Laura Soucek** Models of Cancer Therapies Laboratory at the Vall d'Hebron Institute of Oncology (VHIO)	**Challenges and opportunities for a MYC inhibitor in cancer treatment**
Oral Session A	**Bioapplications**	
Oral Session B	**Synthesis and Characterization**	
Oral Session C	**Nanofabrication**	
Oral Session D	**Energy and Environment**	

Friday 26th of November 2021		
Plenary Talk	**Dr. Montse Pont** ALBA Synchrotron	**ALBA II, the upgrade project of the ALBA Synchrotron**
Workshop 1	**Dr. Salvador Ferré Benedicto** Universitat de Vic (UVic)	**Scientific Communication**
Poster Session		
Round Table	**Dr. Clara Barker** Centre for Applied Superconductivity at Oxford	**Diversity in STEM disciplines**
	Dr. Carmen Botella School of Engineering of the Universitat de València	
	Prof. Xavier Roque Universitat Autonoma de Barcelona (UAB)	
	Prof. Gemma Garcia Universitat Autonoma de Barcelona (UAB) / AMIT-Cat	
Workshop 2	**Dr. Xavier Borrisé** IMB-CNM-CSIC	**Into the Nanolaboratory!**
	Mr.Albert Guerrero IMB-CNM-CSIC	
Plenary Talk	**Prof. César de la Fuente** University of Pennsylvania	**Machine Biology for Infectious Diseases**

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PLENARY TALK

Prof. Xavier Obradors

Institut de Ciència de Materials de Barcelona (ICMAB CSIC)



Xavier Obradors is a research professor and Director of the Institut de Ciència de Materials de Barcelona (ICMAB-CSIC). He earned his degree in physics (1978) and his PhD in physics (1982) at the Universitat de Barcelona, and materials science (1983) at the Université Scientifique et Médicale de Grenoble (France).

His research is focused on materials preparation with controlled micro/nanostructures and the comprehension of the physical mechanism underlying the superconducting, magnetic, and electronic properties of nanostructured materials, particularly complex oxides. He has published more than 750 articles, which have received over 16700 citations (h-index of 59) (Google scholar). The main recent accomplishments have been in the field of high current superconductors, particularly in materials development based on high throughput low cost chemical solution deposition (CSD) methods. He has received several awards: Member of the Royal Academy of Science and Arts of Barcelona (1998); Medal to the scientific achievements Narcís de Monturiol (1999); Fellow of the Institute of Physics (1999); National Prize Blas Cabrera of Physical Sciences, Materials and Earth studies (2003); Chevalier dans l'Ordre des Palmes Academiques (2005); ENDESA-NOVARE Prize to Energy Efficiency (2007); Leibniz Medal of the Institut of Solid State and Materials Research, Desdren (2016); City of Barcelona Prize to Experimental Science and Technology, Barcelona (2016).

He has coordinated many national and international projects, among them the Severo Ochoa Excellence Award of ICMAB "Smart Functional Materials for social grand challenges" (FUNMAT).

Clean Energy Transition: What Can We Expect from Superconductivity?

Anthropogenic global warming is the most serious concern that humanity faces nowadays. It is affecting all aspects of society spanning energy, healthcare, agriculture and economy, so research and development to create novel technologies to accelerate the clean energy transition is one of the highest goals at present.

Nanoscience and nanotechnology have established new paradigms to generate knowledge and materials with the capacity to radically transform many technological sectors, particularly those involved in the clean transition. Therefore, taking into account that technologies are always limited by the materials available, high-performance nanomaterials are destined to become the keystone for clean energy.

In this context, what can we expect from superconductivity? Superconductivity is a key technology of the 21st century, boosted by the discovery of high temperature superconductors (HTS), that will lead to drastic changes in the way electricity is generated, transported, distributed and used, as well as in transportation (airplanes, ships).

On the one hand, current electrical systems will be more efficient (cables, motors, transformers, generators, etc.), thus contributing to energy savings. On the other hand, new systems and technologies will appear, which we do not currently have, allowing us to use more intelligently the electrical energy. These new technologies include fusion reactors, energy storage systems and fault current limiters that will ensure the safe and reliable electricity grids adapted to renewable energies. Additionally, HTS will also boost applications in other sectors, such as biomedicine, high energy physics or transportation.

But HTS are nanomaterials that need to be thoroughly developed for this new scenario to become a reality. The manufacture of efficient HTS wires requires the development of new methodologies in which the materials have a very particular internal nanostructure. In short, it is a matter of finding cost-effective materials manufacturing methodologies, for kilometer lengths, keeping control of their internal structure at the nanometer scale, and using at best the physical properties of HTS.

In this talk I will present the present worldwide scenario of superconductivity research where the colossal challenge of reaching a clean energy transition is being explored.

- Need of clean energy transition: sustainability. Distribution of energy use. CO2 generation (per capita)
- Roadmaps towards GHG neutrality (2050). Paris agreement.
- Other industries: textile, agriculture, woods, efficiency.
- Population evolution, emigration
- The new paradigms: electricity and renewable fuels. It is a materials party!
- Challenges: land and sea use; critical raw materials; recycling
- Electricity: generation, transport and distribution, storage, final use
- Transportation: aviation, maritime, trains (MAGLEV)
- Synergy between solar fuels (chemistry) and electricity
- Why superconductivity?. Low losses, efficiency, high magnetic fields, high currents
- HTS materials: challenges
- Generation: 1/ Wind generators (HTS); 2/ Fusion (LTS and HTS)
- Transmission and distribution: 1 / cables; 2/ Fault current limiters
- Storage: SMES
- Transportation:
  - Aviation:: motors, cables
  - Maritime: motors, generators, FCL, cables
  - MAGLEV
- Other outputs: High Energy Physics, Biomedecine (NMR, MRI, proton therapy), Environment (magnetic separation)
- Challenges in HTS materials: cost/performance under different working situations (low, medium, high magnetic fields)
- Conclusions

PLENARY TALK

Dr. Laura Soucek



Models of Cancer Therapies Laboratory at the Vall d'Hebron Institute of Oncology (VHIO)

Dr. Laura Soucek is the principal investigator of the Models of Cancer Therapies Laboratory at the Vall d'Hebron Institute of Oncology (VHIO), Co-Founder and Chief Executive Officer (CEO) of Peptomyc S.L., Associate Professor at Universitat Autónoma de Barcelona (UAB) and ICREA Research Professor.

Her remarkable scientific career and research on Myc oncoprotein and its inactivation by inhibitory cell-penetrating miniproteins for cancer treatments have been recognized trough several prestigious national and international grants (FERO fellowship, ERC Consolidator grant, two ERC Proof of Concept grants and a Worldwide Cancer Research grant), making her a leading figure in that field.

In 1998, when she was still an undergraduate student, she designed Omomyc, which has been recently approved by the Spanish Agency of Medicines and Medical Devices (AEMPS) to be tested in the first-in-human Phase I/II clinical trial. It currently emerges as the first disruptive Myc inhibitor preventing tumor growth in a safe way, only causing mild and reversible side effects.

Challenges And Opportunities for A MYC Inhibitor in Cancer Treatment

MYC is one of the most wanted targets for therapeutic intervention in cancer, having a key role in driving and maintaining most, if not all, human tumors. Despite this indisputable therapeutic opportunity, MYC has long been perceived as “undruggable” for its intrinsically disordered nature and fear of catastrophic side effects in normal tissues. Indeed, to date, there is still no MYC inhibitor in the clinic.

We previously designed a dominant negative form of MYC called Omomyc and used its conditional transgenic expression to inhibit MYC function both in vitro and in vivo, demonstrating a potent therapeutic impact in various mouse models of cancer, while causing only mild, well-tolerated and reversible side effects. Importantly, we recently showed that the purified Omomyc mini-protein displays unexpected cell-penetrating properties and can be delivered directly to tissues or by systemic administration to target tumors in different tissues and harboring various oncogenic mutation profiles. These features give the Omomyc mini-protein great potential for clinical development and application in multiple oncological indications. In fact, clinical trials Phase I/IIa have begun in 2021 and are currently ongoing to test Omomyc safety and efficacy in patients with solid tumors.

SESSION A - BIOAPPLICATIONS

A01

Antitumoral nanoparticles with multiple activities, a close reality

Eric Voltà-Durán [1,2,3], Naroa Serna [1,2,3], Laura Sánchez-García [1,2,3], Anna Aviñó [3,4], Julieta M. Sánchez [1,2,5], Hèctor López-Laguna [1,2,3], Olivia Cano-Garrido [1,6], Isolda Casanova [3,7,8], Ramón Mangues [3,7,8], Ramon Eritja [3,d], Esther Vázquez [1,2,3], Antonio Villaverde [1,2,3], Ugutz Unzueta [2,3,7,8]

1 *Institut de Biotecnologia i de Biomedicina, Universitat Autònoma de Barcelona, Bellaterra, 08193 Barcelona, Spain*

2 *Departament de Genètica i de Microbiologia, Universitat Autònoma de Barcelona, Bellaterra, 08193 Barcelona, Spain*

3 *CIBER de Bioingeniería, Biomateriales y Nanomedicina (CIBER-BBN), Bellaterra, 08193 Barcelona, Spain*

4 *Institute for Advanced Chemistry of Catalonia (IQAC), CSIC, 08034 Barcelona, Spain*

5 *Instituto de Investigaciones Biológicas y Tecnológicas (IIBYT) (CONICET-Universidad Nacional de Córdoba). ICTA & Cátedra de Química Biológica, Departamento de Química, FCEFyN, UNC. Av. Velez Sarsfield 1611, X 5016GCA Córdoba, Argentina*

6 *Nanoligent SL, Edifici Eureka, Universitat Autònoma de Barcelona, Bellaterra, 08193 Barcelona, Spain*

7 *Biomedical Research Institute Sant Pau (IIB Sant Pau), Sant Antoni M ªClaret 167, 08025 Barcelona Spain*

8 *Josep Carreras Leukaemia Research Institute (IJC), Barcelona, Spain*

eric.voltaduran@gmail.com

Antitumoral nanoparticles with multiple activities, a close reality. The major drawback of conventional anticancer treatments using pharmaceuticals (chemotherapy) is that they promote damage in cells and organs that are not affected by the disease. Because of this, the development of tumor-targeted therapies represents an opportunity to selectively destroy tumoral cells without causing off-side effects in the rest of the body. To this end, the group of Nanobiotechnology (NBT) from the Department of Genetics and Microbiology and the Institut de Biotecnologia i Biomedicina (IBB-UAB), in close collaboration with the group of Oncogènesi i Antitumorals (GOA) from the Institut de recerca de l'Hospital de la Santa Creu i Sant Pau (IIB-Sant Pau), develops a new concept of pharmaceuticals based on protein nanoparticles generated with bacterial expression systems. These drugs are selective for metastatic stem cells (those responsible of cancer propagation, recurrence and bad prognosis) that overexpress in their surface the CXCR4 receptor, present in 23 distinct types of cancer. Using a precise protein engineering, we generate multi-functional protein nanoparticles that remain in the bloodstream for a long time and selectively enter and destroy metastatic stem cells, thus contributing to stop cancer progression. In the last years, we have employed two main strategies in the development of antitumoral protein nanoparticles. On one side, toxins from bacterial origin (Pseudomonas aeruginosa exotoxin A and Corynebacterium diphtheriae toxin), venoms or other death-inducer proteins have been introduced in the original targeted-protein design, conferring the product an antitumoral intrinsic activity. On the other side, current chemotherapeutics, already used in clinics in non-targeted approaches,

have been chemically linked to inert targeted nanoparticles, directing their effect to the tumor. Both strategies are covered by intellectual property rights. Recently, we have explored the possibility of combining both strategies to generate intrinsically toxic nanoparticles loaded with conventional chemotherapeutics in a single pharmacological entity. This way, we seek to potentiate their antitumoral effect and face the appearance of resistances in the tumor. In this initial step, the concept proposed has been demonstrated as fully feasible, as stable nanoparticles that contain both the toxin and the loaded chemotherapeutics were generated, though their toxic effect did not improve in CXCR4+ tumor cell lines. Nevertheless, thanks to this research, the main bottleneck of the technology has been identified. A precise control of drug binding site is needed to maintain the antitumoral capacity of targeted bacterial toxins, which act at the same time as active principle and anchoring site for chemical drugs. This novel platform, that recruits in a single pharmacological entity different therapeutic actions may open a broad investigation field in the design of antitumoral drugs.

Eric Voltà-Durán, Naroa Serna, Laura Sánchez-García, Anna Aviñó, Julieta M. Sánchez, Hèctor López-Laguna, Olivia Cano-Garrido, Isolda Casanova, Ramón Mangues, Ramon Eritja, Esther Vázquez, Antonio Villaverde, Ugutz Unzueta. (2021) Design and engineering of tumor-targeted, dual-acting cytotoxic nanoparticles Acta Biomaterialia,V. 119, Pg.312-322 https://doi.org/10.1016/j.actbio.2020.11.018

A02

Impact of hierarchical Quatsome-RGD nanostructured surfaces on integrin-mediated cell adhesion

Marc Martínez-Miguel [1,2], Miquel Castellote-Borrell [1], Mariana Köber [1,2] , Adriana R. Kyvik [1,2] , Judit Tomsen-Melero [1,2] , Guillem Vargas-Nadal [1] , Jose Muñoz [1] , Daniel Pulido [2, 3] , Edgar Cristóbal-Lecina [2,3] , Solène Passemard [1] , Miriam Royo [2,3] , Marta Mas-Torrent [1,2] , Jaume Veciana [1,2] , Marina I. Giannotti [2,4,5] , Judith Guasch [1,2, 6] , Nora Ventosa [1.2] , Imma Ratera [1.2]

1 Barcelona Institute of Materials Science (ICMAB-CSIC), UAB Campus, 08193, Bellaterra, Spain

2 Biomedical Research Networking Center on Bioengineering, Biomaterials and Nanomedicine (CIBER-BBN), Spain

3 Institute of Advanced Chemistry of Catalonia (IQAC-CSIC), 08034, Barcelona, Spain

4 Nanoprobes and Nanoswitches group, Institute for Bioengineering of Catalonia (IBEC), The Barcelona Institute of Science and Technology (BIST), 08028, Barcelona, Spain

5 Department of Materials Science and Physical Chemistry, University of Barcelona, 08028, Barcelona, Spain

6 Dynamic Biomimetics for Cancer Immunotherapy, Max Planck Partner Group, ICMAB-CSIC, Campus UAB, 08193, Bellaterra, Spain

mmartinez@icmab.es

The study of the RGD peptide, found in many extracellular matrix proteins, has allowed to produce a wide range of cell adhesive surfaces. Although the impact of RGD density and spacing at the nanoscale has already shown an influence on cell

adhesion, the study of its hierarchical nanostructuration is still rather unexplored. In this work, a colloidal system named Quatsomes, based on fluid nanovesicles formed by self-assembling of cholesterol and surfactant molecules, has been devised as a template to achieve hierarchical nanostructures of the RGD peptide on surfaces. To this end, RGD-functionalized Quatsomes were covalently anchored to planar gold surfaces in a state of quasi-suspension. RGD-Quatsome decorated surfaces greatly enhanced cell adhesion in comparison to surfaces with homogeneously distributed RGD. A multi-technique characterization of the surface confirmed the presence of anchored Quatsomes and remarked the effect of the nanostructuration of the RGD peptides regarding the cellular response.

A03

Polypyrrole nanoparticles for cardiac resynchronization & evaluation in C. elegans

Sumithra Yasaswini Srinivasan[1], N. B. Cases[2, 3], A. Laromaine[1]

1 Institut de Ciència de Materials de Barcelona (ICMAB), UAB, Spain

2 ALBA Synchrotron, Cerdanyola del Vallès, Spain

3 Universitat de Autoericnoma de Barcelona, Spain

ssumithra@icmab.es

Cardiac arrhythmia is caused by irregular pumping due to a dysregulation in the voltage-gated cation channels. As much as 40% of deaths by cardiovascular deaths occur due to cardiac arrhythmia (CA) and 90% of patients with existing cardiovascular conditions suffer arrhythmia. Since CA can be caused by several gene mutations, personalized mutation-specific models are indispensable for testing new cardiac drugs and nanomaterials. However, using a gene-specific animal model for each type of cardiac arrhythmia is complicated, expensive and time-consuming. Caenorhabditis elegans (C. elegans) share 60% genetic homology to humans, are optically transparent enabling facile visualization and exhibit short life span and fast reproduction cycle. It is also easy to produce rapid construction of transgenic and transformed animals, perform large-scale screening with RNAi knockdowns, and the mutants can be frozen and maintained indefinitely. Interestingly, although C. elegans do not possess a heart, they possess pharynx, a pumping organ with molecular mechanism much similar to humans´ cardiac pumping involving voltage gated Ca2+ channels responsible for transient Ca2+ conduction. In this work, we aim to establish C. elegans as a simple and fast small animal model for screening toxic profiles and anti-arrhythmic efficiency of drugs and nanomaterials for arrhythmia such as the polypyrrole nanoparticles. Polypyrrole nanoparticles (Ppy NPs), being electrically conducting are shown to synchronize irregular cardiac rhythms in-vitro by regulating the cardiac electrical impulses. In this work we will present synthesis and characterization of Ppy NPs, systemic toxicity of Ppy NPs in C. elegans, effect of Ppy NPs in pharynx pumping rate in three different strains of C. elegans.

A04

A novel electronic tongue based on molecularly imprinted polymers for pharmaceutical analysis

Mingyue Wang[1], Xavier Cetó[1] and Manel del Valle[1]

1 Sensors and Biosensors Group, Department of Chemistry, UAB

manel.delvalle@uab.es

The demand for accurate and rapid pharmaceutical analysis has progressively increased because of drugs' negative effects, especially in cases of overdosing. This work reports a facile and general strategy for the synthesis of three different molecularly imprinted polymers (MIPs) and their usage in a sensor array to construct a novel electronic tongue for the simultaneous determination of paracetamol, ascorbic acid and uric acid mixtures. The MIPs film was characterized by cyclic voltammetry, electrochemical impedance spectroscopy, scanning electron microscopy and energy-dispersive X-ray spectrometry. Especially, p-toluenesulfonate anion (pTS-) was integrated into the polypyrrole (PPy) MIPs backbone as counter-ion. Serving as the functional interface for stable integration, pTS- /PPy MIPs rendered the tailored physicochemical properties and the prominent electrochemical performance. Taking the complementary advantages from MIPs structures and electronic tongue sensing platforms, a pTS- /PPy MIPs sensor array exhibited superb sensitivity, selectivity, and a wide detection range in the simultaneous determination of the three active pharmaceutical ingredients (APIs). Lastly, the applicability of the developed approach was assessed through the analysis of pharmaceutical tablets with satisfactory agreement between expected and obtained values by artificial neural networks (ANNs) (R2>0.987).

A05

Robust transcriptional indicators of plant immune cell death revealed by spatio-temporal transcriptome analyses

Jose Salguero Linares[1], Irene Serrano[2], Nerea Ruiz-Solani[1], Marta Salas-Gómez[1], Ujjal Jyoti Phukan[1], Victor Manuel González[1], Martí Bernardo-Faura[1], Marc Vallsa[1,2], **David Rengel**[2,3], **Nuria S. Coll**[1,4]

1 Centre for research in agricultural genomics, UAB

2 LIPM, Universite de Toulouse, INRA, CNRS, 84195 Castanet-Tolosan, France

3 INRAE, GeT-PlaGe, Genotoul, 31326 Castanet-Tolosan, France (doi: 10.15454/1.5572370921303193E12)

4 Department of Genetics, Universitat de Barcelona, 08028 Barcelona, Spain

j.salguerolinares16@gmail.com, nuria.sanchez-coll@cragenomica.es, david.rengel@ipbs.fr

Recognition of a pathogen by the plant immune system often triggers a form of regulated cell death traditionally known as the hypersensitive response. This type of immune cell death occurs precisely at the site of pathogen recognition, and it is restricted to a few cells. Extensive research has shed light into how plant immune receptors are mechanistically activated. However, a central key question remains largely unresolved: how does cell death zonation take place and what are the mechanisms that underpin this phenomenon? As a consequence, bona fide transcriptional indicators of immune cell death are lacking, which prevents gaining a deeper insight of its mechanisms before cell death becomes macroscopic and precludes any early or live observation. We addressed this question using the paradigmatic Arabidopsis thaliana–Pseudomonas syringae pathosystem, by performing a spatio-temporally resolved gene expression analysis that compared infected cells that will undergo immune cell death upon pathogen recognition vs by-stander cells that will stay alive and activate immunity. Our data revealed unique and time-dependent differences in the repertoire of differentially expressed genes, expression profiles and biological processes derived from tissue undergoing immune cell death and that of its surroundings. Further, we generated a pipeline based on concatenated pairwise comparisons between time, zone and treatment that enabled us to define 13 robust transcriptional immune cell death markers. Among these genes, the promoter of an uncharacterized AAA-ATPase has been used to obtain a fluorescent reporter transgenic line, which displays a strong spatio-temporally resolved signal specifically in cells that will later undergo pathogen-triggered cell death. In sum, this valuable set of genes can be used to define those cells that are destined to die upon infect immune cell death-triggering bacteria, opening new avenues for specific and/or high-throughput techniques to study immune cell death processes at a single-cell level.

A06

Riboflavin-citric conjugate for enhanced MRI contrast and cellular uptake of SPIONs in breast cancer cells

Wid Mekseriwattana[1,2], Pablo Guardia[2], Anna Roig[2], Kanlaya Prapainop Katewongsa[1,3]

1 School of Materials Science and Innovation, Faculty of Science, Mahidol University, Bangkok 10400, Thailand

2 Institut de Ciència de Materials de Barcelona (ICMAB CSIC), Campus UAB, Bellaterra 08193, Spain

3 Department of Biochemistry, Faculty of Science, Mahidol University, Bangkok 10400, Thailand

wmekseriwattana@icmab.es

Female breast cancer is the most prevalent type of cancer worldwide, according to a report in 2020 (1). Different types of riboflavin (Rf)-associated proteins were found to be overexpressed in breast cancer patients (2, 3); thus, several research efforts use Rf-vitamin and its derivatives as directing ligands to target drug delivery nanoparticles to the cancer cells. Although positive results have been reported in nanoparticle delivery, utilizing of Rf is hindered by limited

hydrophilicity and lack of reactive functional groups which affect strongly on the synthesis and stability of the nanoparticles. As such, complex synthesis routes are required for modification of Rf. Therefore, this work aims to develop a novel Rf-based ligand synthesized through simple synthesis, to provide both stabilizing effect and ability to enhance breast cancer uptake for superparamagnetic iron oxide nanoparticles (SPIONs), which are biocompatible nanoparticles with intrinsic properties suitable for both diagnosis and treatment of cancers. The ligand was formulated by conjugation between Rf and citric acid through a one-step reaction, followed by coating on the SPIONs through complexation of the citrate moieties and the Fe atoms. The stability of the Rf-SPIONs was evaluated in terms of aqueous hydrodynamic diameter and zeta-potential, in comparison with citrate-coated SPIONs. Breast cancer targeting property was investigated by binding study between Rf-SPIONs with riboflavin carrier protein (RCP), a protein overexpressed in breast cancer tissues, using isothermal titration calorimetry and in vitro cellular uptake assays with MCF-7 breast cancer cell line as a model. Finally, magnetic resonance imaging (MRI) and magnetic hyperthermia (MH) performances of the Rf-SPIONs were measured to evaluate the potential of the system to be used as a theranostic drug delivery platform. With the citrate-Rf ligand, Rf-SPIONs showed a hydrodynamic diameter of 100 nm in water with a narrow polydispersity index. The size was maintained for at least 7 days upon dispersion, reflecting good aqueous stability of the nanoparticles. The Rf-SPIONs showed specific entropy-driven binding with RCP. No toxicity toward the cells was observed when treated with SPION concentrations of up to 200 µg mL-1. Prussian blue staining and flow cytometry both showed a superior cellular internalization behavior of the Rf-SPIONs at physiological temperature. At 4˚C, cellular uptake of the Rf-SPIONs drastically dropped as a consequence of the inhibition of cellular activity, suggesting an active transport cellular internalization pathway. Evaluation of magnetic responses suggested excellent MRI and moderate MH performances. Therefore, the Rf-SPIONs have been proven as a potent system to be developed as a breast cancer theranostic platform. Also, the citrate-Rf has shown a property to activate cellular internalization of nanoparticles in breast cancer cells, therefore, could be possible to apply to other nanoparticle systems in the future.

A07

Evaluating bacterial cellulose as a dietary fiber in the nematode Caenorhabditis Elegans

Amanda Muñoz-Juan[1], Soledad Roig-Sanchez[1], Núria Benseny-Cases[2], Anna Laromaine[1]

1 Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Catalonia, 08193 Bellaterra, Spain.

2 Biophysics Unit, Department of Biochemistry and Molecular Biology, Universitat Autònoma de Barcelona (UAB)

amunoz@icmab.es

Cellulose is getting attraction in the food and pharmaceutical industry due to its biocompatibility, degradability, hydrophobicity, chirality, and easy functionalization [1]. There is evidence that celluloses modify gut motility and nutrients absorption [2]. Cellulose´s water holding capacity is ideal for drug delivery systems based on it but, it is necessary a better knowledge of cellulose's effects on organisms. Here we proposed Caenorhabditis elegans (C.

elegans) as a simple animal model to study the biointeraction of cellulose, in specific, bacterial nanocellulose (BC). BC is purer than vegetal cellulose and has a different nanostructure, which increases its chance in the biomedical and food field. Firstly, we biosynthesize BC fibers1 and characterized them physiochemically. In the biological characterization, we expose BC to C. elegans and we localize it inside the worms' intestine; then survival rate, growth, and reproduction were evaluated as the principal toxicological endpoints. Moreover, we performed a RNAseq analysis and observed which routes were up or downregulated by BC uptake. Finally, we assessed the impact of BC ingestion in the lipid metabolism of C. elegans using two complementary methodologies: Oil-red-O (ORO) staining and µFourier-transform infrared spectroscopy (µFTIR). This work confirmed the low toxicity of BC, revealed for the first time which routes are affected by the BNC's uptake and shown a reduction of lipid oxidation due to the presence of BNC in the diet. Altogether, these results validated the use of BC as a food additive and its potential as drug delivery carrier. C. elegans is a proper animal model for the evaluation of polysaccharides' biointeraction and pave the way for the evaluation of cellulose derivatives and drug delivery systems economically and efficiently.

SESSION B - SYNTHESIS AND CHARACTERIZATION

B01

Electromechanical response of epitaxial Lead Zirconate thin films

Saptam Ganguly[1], Pablo Vales-Castro[1], Ying Liu[1], Gustau Catalan[1,2]

1 Catalan Institute of Nanoscience and Nanotechnology (ICN2-CSIC)

2. ICREA Institució Catalana de Recerca i Estudis Avançats), Barcelona 08010, Spain

saptam.ganguly@icn2.cat gustau.catalan@icn2.cat

Antiferroelectrics have been suggested as the functional element of many significant technological applications that include micro positioners, energy storage devices, electro-optic devices, and more recently the possibility of solid state cooling owing to their large negative electrocaloric effect [1-6]. However, in order to use antiferroelectrics in potential actuator devices we need a detailed understanding of their electromechanical response that is still lacking so far [7-9]. In this work, we use the archetype antiferroelectric Lead Zirconate ($PbZrO_3$, PZO) as our model system and we study the electric-field-induced strain in PZO thin films. With the aid of Digital Holographic Microscopy (DHM) we can precisely quantify the total strain induced in the film and we can distinguish the three different mechanisms that induce strain during the application of an electric field: electrostriction, lattice expansion during the antiferroelectric-ferroelectric phase transition and the piezoelectricity emerging in the ferroelectric phase after the phase transition is completed. Such a precise determination of the different origins of strains further allows to observe a general tendency of the PZO films to stabilize a meta-stable ferroelectric phase upon voltage cycling. Keywords: Antiferroelectric; Digital Holographic Microscopy; Electromechanical Response.

B02

Synthesis and physic chemical characterization of a new hybrid polyoxovanadate (C6N2H9)4[H2V10O28]4H2O.

Idia Msaadi[1], Ali Rayes[1],Monica Benito[2], Elies Molins[2] .,Brahim Ayed[3]

1 Laboratory of Research, Catalysis and Materials for the Environment and Processes, LRCMEP, (LR19ES08), Faculty of Sciences of Gabès, University Campus, 6072 Gabès, Tunisia
2 Institute of Materials Sciences of Barcelona (ICMAB-CSIC) Compus UAB, 08193 Bellaterra, Spain
3 University of Monastir, Laboratory of Physico-chemistry of Materials LR01ES19, Faculty of Sciences, Tunisia

msaadiidia@gmail.com

New hybrid composite materials, (C6N2H9)4[H2V10O28].4H2O, have been synthesized from acidified aqueous solution and characterized by IR, UV-visible spectroscopies, single crystal

X-Ray diffraction and thermal analysis. The asymmetric unit of (C6N2H9)4[H2V10O28].4H2O is composed of one half decavanadate [H2V10O28]2-, two picolylamonium cations and four water molecules. The cohesion of the crystal packing is provided by a complex network of N-H ••• O, Ow-H •••O and O-H •••Ow hydrogen bonds involving water molecules and organic molecules as well as Vander Waals interactions for the connection between the organic molecules. A fluorescence measurement of the title compound is also investigated in detail. The presence of organic cations and water molecules are confirmed by IR spectra. The UV-vis diffuse reflectance spectrum shows that the hybride material exhibit semiconducting behavior with an optical band gap of 2.33 eV.

B03

Temporal regulation luminescence of hydrophobic mixed Eu^{3+}/Tb^{3+} Metal-Organic Frameworks for anticounterfeiting

Zhen Li[1], Claudio Roscini[2], Rosario Núñez[1], Mark E. Light[3], Eliseo Ruiz[4], Francesc Teixidor[1], Clara Viñas1, Daniel Ruiz-Molinal[2], José2 Giner Planas[1]

1 Institute of Materials Science of Barcelona (ICMAB-CSIC)

2 Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC, and The Barcelona 3 Institute of Science and Technology (BIST), Campus UAB, Bellaterra, Barcelona 08193, Spain

3 Department of Chemistry, University of Southampton, UK.

4 Departament de Química Inorgànica i Orgànica and Institut de Recerca de Química Teòrica i Computacional, Universitat de Barcelona, Spain.

jginerplanas@icmab.es

Luminescent Lanthanide coordination polymers or metal–organic frameworks (Ln-CPs or -MOFs) have been shown to exhibit relevant optical properties of interest for practical applications though its implementation still remains a challenge. Before practical applications, Ln-MOFs must be not only water stable, but printable, easy to prepare and high yield. Herein, we design and synthesize a series of EuxTb1-x CPs using a highly hydrophobic ligand mCBL1: 1,7-di(4-carboxyphenyl)-1,7-dicarba-closo-dodecaborane. The new materials are stable in water and at high temperature. Tunable emission from green to red, energy transfer (ET) from Tb3+ to Eu3+ and temporal regulation of the series of mCB-EuxTb1-x doped MOFs are reported. An outstanding increased of 239% of the quantum yield of mCB-Eu (20.5 %) in the mixed mCB-Eu0.1Tb0.9 (69.2%) is achieved, along with an increased and tunable lifetime luminescence, all these promoted by a highly effective ET process. We report a convenience method to prepare mixed metal Eu/Tb CPs and printable from water inks for potential applications, among which anticounterfeiting has been selected as a proof-of-concept. Keywords: Luminescent Lanthanide coordination polymers, hydrophobic carborane-based ligands, water stability, temporal regulation luminescence, anticounterfeiting materials.

B04

Crystal structure and Optical properties of (3-ampH$_2$)BiCl$_5$ H$_2$O

Selma Msaoura[1], Ali Rayes[2] and Ammar Houas[3]

1 Faculty of Sciences of Gabes (FSG)

2 Laboratory of Research, Catalysis and Materials for the Environment and Processes, LRCMEP, (LR19ES08), Faculty of Sciences of Gabes, University Campus, 6072 Gabes, Tunisia.

3 Laboratory of Research, Catalysis and Materials for the Environment and Processes, LRCMEP, (LR19ES08), Faculty of Sciences of Gabes, University Campus, 6072 Gabes, Tunisia.

salma.msawra@fsg.u-gabes.tn

Crystal structure and Optical properties of (3-ampH$_2$)BiCl$_5$ H$_2$O Selma Msaoura, Ali Rayes and Ammar Houas -Catalysis and Materials Research Laboratory for the Environment and Processes (LRCMEP), University of Gabès, Tunisia. Abstract. The new compound (3-ampH$_2$) [BiCl$_5$].H$_2$O have been prepared by reaction of (Bi(NO$_3$)$_3$), concentrated HCl (37%) and 3-picolylamine at room temperature and characterized by Infrared, single X-ray diffraction, Hirshfeld surface analysis, thermal analysis, optical absorption and photoluminescence measurements. In the IR spectrum there are bands in the 3500-2900 cm-1 correspond to H2O, NH$_3$ and CH$_2$ to stretching vibrations. The for bands observed in the range from 2944 cm-1 to 2137 cm-1 assigned to the asymmetric and asymmetric stretching vibrations of CH$_2$, and the bands appeared 1557, 1501, 1475 cm-1are assigned to asymmetric and symmetric bending vibrations of CH$_2$. The band observed at 1613 cm-1 assigned to the stretching vibration of the aromatic C=N. Single X-ray diffraction shows that the title compound crystallizes in triclinic system with P-1 space group with a=7.8491(3), b=9.7284(4), c=10.5000(5), α=67.394(2), β=87.635(2), γ=75.493(2), Z=2, and V=715.21(5). The structure is formed by isolated [Bi$_2$Cl$_{10}$]4- units composed of two [BiCl$_5$]2- octahedron sharing two vertices, di-protonated organic cations and water molecules located between the two sublatices. The structure cohesion is performed by hydrogen bonds between these two entities. Hirshfeld surface and the two-dimensional fingerprint analysis confirm that the H···Cl/Cl···H, H···O/O···H, H···C/C···H hydrogen bonds and H···H Van Der Waals interactions had the most contribution for the structure build and stability. This result is coherent with the single X-ray diffraction. The Optical measurement given that the little compound is a semi-conductor which presents a blue-green luminescence.

B05

Iridium oxide redox gradient material: Operando X-Ray absorption of Ir gradient oxidation states during IrOx bipolar electrochemistry

L. Fuentes-Rodríguez [1,2], Ll. Abad[2], Laura Simonelli[3], D. Tonti[1], N. Casañ-Pastor[*1],

1 Institut de Ciència de Materials de Barcelona-CSIC, Campus UAB, 08193 Bellaterra, Barcelona, Spain

2 Institut de Microelectrònica de Barcelona-CNM-CSIC, Campus UAB, 08193 Bellaterra, Barcelona, Spain

3 ALBA Synchrotron Light Facility, Carrer de la Llum 2-26, 08290 Cerdanyola del Vallès, Spain

lfuentes@icmab.es

When conducting materials are immersed in an electrolyte, induced dipoles and bipolar electrochemistry processes change the electrochemical cell characteristics. Simple polarization effects or electric percolation had not been sufficient to explain those changes in suspensions, since those changes occur well below the electronic percolation limits. This work shows that a significant lower resistance of the cell and charge transfer effects are present even for a discrete number of non-mobile conducting pieces inserted unconnected in the blank electrolyte. Using macroscopic conducting immersed pieces, a physical mediation due to transport through the induced dipoles is observed and if redox species exist, is enhanced. The combination is considered a physicochemical mediation. Shape or geometry, as well as size of the conducting pieces and occupation of the main field lines are significant. It is relevant that the effects observed are parallel to the previously reported for carbon suspensions and slurries, and that no electronic percolation, or induced particle ordering are needed to reach those large effects.

B06

Advanced STEM Characterisation of SiGe/Ge Quantum Wells for Quantum Computing

Marc Botifoll[1], Carla Borja[1], Daniel Jirovec[2], Kushagra Aggarwal[2], Georgios Katsaros[2], Jordi Arbiol[1,3]

1 Catalan Institute of Nanoscience and Nanotechnology (ICN2-CSIC)

2 Institute of Science and Technology Austria, Am Campus 1, 3400 Klosterneuburg, Austria

3 ICREA, Pg. Llus Companys 23, 08010 Barcelona, Catalonia, Spain

marc.botifoll@icn2.cat

Quantum computing is thought to be one of the main technological revolutions to occur in the current century. It will become ubiquitous in our society providing with powerful tools to solve scientific problems in diverse fields such as chemistry and drug design, biomedical research and personalised medicine, and engineering, among others. Towards achieving quantum

processing units, germanium is an outstanding platform to create well-controlled quantum dots given its high hole mobility and low effective mass. In this study, we have explored the materials science implications behind the creation of a Ge-based Josephson field-effect transistor (JoFET) [1] and a singlet-triplet hole spin qubit [2]. HAADF-STEM was used to get atomic resolution micrographs of the misfit dislocation-free Ge quantum wells (QW) and their interfaces with the SiGe surrounding layers, and crystalline Al and Nb metallic contacts, when present. We computed the elastic strain by a correlative study between geometrical phase analysis (GPA) and quantitative-EELS and X-ray diffraction (XRD). We proved the feasibility of extracting reliable quantitative compositional information by means of core-loss EELS despite plural scattering when complementary reference values are provided (e.g. XRD). We used this precise compositional information to correlate the relative lattice displacements unveiled by GPA to the strain to which every region of the device has undergone. In conclusion, we have applied a systematic structural-compositional correlative characterization to state-of-the-art Ge-based devices for hole spin qubits generation in an ongoing study aiming for an optimized quantum performance.

B07

Sapphire template preparation for the epitaxial growth of MoS2 thin films

C. M. Schaefer[1], A. T. Hoang[2], J. Caicedo Roque[1], J. Santiso[1], J.-H. Ahn[2], J.A. Garrido[1,3]

1 Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Bellaterra (Barcelona), Spain

2 Yonsei University, Department of Electrical & Electronic Engineering, Seoul, Rep. of Korea

3 Catalan Institution for Research and Advanced Studies (ICREA), Barcelona, Spain

christian.schafer@icn2.cat

Sapphire (α-Al_2O_3) is a crystalline substrate widely used for epitaxial thin film growth with industrial importance in metal-organic chemical vapor deposition (MOCVD) of traditional III-V semiconductors, such as GaN, [1]. Recently, it has attracted great interest as a substrate for the van der Waals (vdW) epitaxy of single-crystalline layers of two-dimensional (2D) transition-metal dichalcogenide (TMD) semiconductors, such as MoS_2. [2] To enable epitaxy, typically, an atomically-smooth, “epi-ready” substrate surface is required, which can be obtained by high temperature annealing (>1000°C) prior to thin film growth. However, sapphire template preparation for 2D vdW epitaxy by engineering surface morphology and chemistry needs further understanding. [3][4]

Here, we employ atomic force microscopy (AFM), contact angle measurements, and reflection high-energy electron diffraction (RHEED) to study the surface of c-plane sapphire with miscut angles of 0.2° and 0.05° under different annealing conditions, such as time, temperature, and atmosphere (O_2-rich compared to H_2-rich). AFM results show that increased temperatures of 1050 to 1200°C and O_2-rich annealing conditions promote the formation of a regularly stepped surface with atomically-smooth terraces, whose width depends on the miscut angle. While annealing in O_2-rich atmosphere results in the O-terminated 1×1 surface, H_2-rich atmosphere at 1200°C leads to the Al-terminated 31×31R9° surface reconstruction. These different sapphire surface treatments provide a platform to investigate MOCVD of MoS_2 thin films, and, finally, we demonstrate epitaxy on sapphire after annealing with optimized conditions.

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SESSION C - NANOFABRICATION

C01

Robust electroactive substrates for surface-enhanced Raman spectroscopy based on overgrown gold-nanoparticle arrays electrodeposited on indium tin oxide

Nerea Gonzalez-Pato,[1,2] Xavier Rodriguez, [1] Nicola Pellizzi,[1] Judith Guasch, [1,2,3] Jaume Veciana, [1,2] Alejandro R. Goñi, [1,4]* Imma Ratera [1,2]*

1 Institute of Materials Science of Barcelona (ICMAB-CSIC)

2 CIBER de Bioingeniería, Biomateriales y Nanomedicina (CIBER-BBN), Spain

3 Dynamic Biomimetics for Cancer Immunotherapy, Max Planck Partner Group, ICMAB-CSIC, Campus UAB, Bellaterra, 08193 Barcelona, Spain

4 ICREA, Passeig Lluís Companys 23, 08010 Barcelona, Spain

ngonzalez@icmab.es

Detection of single molecules and low concentration of analytes is becoming more and more important. Surface Enhanced Raman Spectroscopy (SERS) is a powerful technique, able to detect trace amount of substances, providing chemical information as a unique spectra for each molecule adsorbed on a rough metal surface. Therefore, in biomedicine and biosensors is becoming a prominent tool. Raman spectroscopy is a non-destructive technique, very sensitive and can be performed at room temperature. One of the actual limitations of this technique is the lack of reproducibility of the signal because substrates used as holder of molecules are not easy to reproduce. In this work we have developed a reproducible, uniform and conductive substrate for SERS following an easy and low-cost methodology, in two simple steps. First, we deposit gold nanoparticles on Indium-Tin Oxide (ITO) substrate by Block-Copolymer Micellar Lithography (BCML) technique, creating a quasi-hexagonal pattern that will act as a template. In a second step we grow these nanoparticles by applying an electrochemical pulse, taking advantage of the conductivity of the ITO. This last step allows to have bigger gold nanoparticles and consequently, smaller distances between each particle, increasing the amount of “hot-spots” in the entire surface. These “hot-spots” are responsible for the intensity of the enhancement of the Raman signal. Here we will show how these substrates not only are an improved tool for SER Spectroscopy but also can be used for electrochemical measurements, coupling both techniques and using the substrate for simultaneous SERS and electroactive characterization of molecules. This opens new opportunities to understand better the mechanisms of electrochemical reactions in biochemistry monitoring in-situ reactions.

C02

Fabrication of films with surface hierarchical micro/nano structures for plastic injection molding

Olga Muntada-López[1], P. Sousa [2], J. Llobet [1], C. Sáez [3], N. Lozano [3], A. Francone [4], N. Kehagias [4], C. Sotomayor [4], **F. Perez-Murano** [1].

1 Institute of Microelectronics of Barcelona (IMB-CNM, CSIC), Campus UAB, Bellaterra 08193 Spain

2 International Iberian Nanotechnology Laboratory (INL), Avda. Mestre José Veiga s/n, Braga 4715-330 Portugal

3 EURECAT, Centre Tecnològic de Catalunya, Unit of Polymeric Materials and Processes, Parc

Tecnològic del Vallès, Av. Universitat Autònoma, 23, Cerdanyola del Vallès 08290 (Barcelona),

4 Catalan Institute of Nanoscience and Nanotechnology (ICN2) Campus UAB, Av. de Serragalliners, s/n, 08193 Bellaterra, Barcelona

olga.muntada@imb-cnm.csic.es, Francesc.Perez@csic.es

We present a scalable method for fabricating nanostructured films by plastic injection molding that contain hierarchical micro/nano structures on the surface. We apply this method to the manufacture of plastic parts with three-level surface micro/nano structures that provide superhydrophobic functionality. The process begins with the fabrication of the silicon master stamp that contains the same hierarchical surface structures that will be present in the final plastic piece. After three steps of replication, we obtain plastic films that are incorporated into an injection molding system to manufacture functional micro/nano structured plastic parts at high throughput and low cost.

C03

Facile chemical route for freestanding complex oxides: from the preparation of $Sr_3Al_2O_6$ sacrificial layer to the final oxide membrane properties

Pol Sallés Perramon[1], Alberto Quintana[1], Ignasi Fina[1], Florencio Sanchez[1], Mariona Coll[1]

1 Institute of Materials Science of Barcelona (ICMAB-CSIC)

polsallesp@gmail.com

Complex oxides are of great interest for their rich variety of chemical and physical properties including magnetism, ferroelectricity, multiferroicity, catalytic behavior and superconductivity. Up to date, the preparation of crystalline complex oxide thin films has been mainly limited on substrates that can stand high temperature thermal treatments and on single crystal substrates when epitaxial growth is pursued. These requirements dramatically limit their applicability excluding the possibility to prepare many artificial multilayered architectures to investigate emergent phenomena that arise in thin films and at their interfaces, as well as

fabrication of flexible devices. In the last few years, it has been proved successful the use of water-soluble $Sr_3Al_2O_6$ (SAO) as sacrificial layer to detach perovskite complex oxides from the growing substrate and freely manipulate them. In these cases, in-situ and high vacuum physical deposition techniques have been used. Herein, our goal is to achieve this SAO sacrificial layer for freestanding complex oxides through the use of cost-effective chemical deposition techniques with atomic precision such as Chemical Solution Deposition (CSD) and Atomic Layer Deposition (ALD). First, we have developed a solution-based procedure to prepare high quality textured SAO films, which have been thoroughly investigated by means of XRD, AFM and TEM between others. Then, we have investigated the viability of SAO to transfer oxide membranes ranging from binary oxides to ternary oxides (ferrites, manganites). These oxides have been deposited on SAO by different deposition techniques (CSD, ALD and PLD), and the effect of these deposition techniques on the oxide membrane quality has been compared. The influence of air exposure on SAO degradation to subsequently transfer epitaxy has been carefully studied by means of XPS and RHEED and identified an effective approach to overcome it. Finally, we studied the transfer of oxide membranes to different supports. In short, this work introduces a chemical-based route to prepare freestanding complex oxides tackling the challenges related to this procedure. These results prove that chemical deposition could become an alternative to high vacuum physical deposition techniques, providing simplicity to the process, and therefore making the freestanding complex oxides a step closer to large-scale production.

C04

Effect of the Organic Semiconductor Side Groups on the Structural and Electronic Properties of Their Interface with Dopants

Adara Babuji[1], Francesco Silvestri[1], Linus Pithan[2], Audrey Richard[3], Yves H. Geerts[3], Nir Tessler[4], Olga Solomeshch[4], Carmen Ocal[1] and Esther Barrena[1]

1 Institute of Materials Science of Barcelona (ICMAB-CSIC)

2 European Synchrotron Radiation Facility,38000 Grenoble, France

3 Laboratoire de Chimie des Polymères,Faculté des Sciences, Université Libre de Bruxelles (ULB),1050 Brussels, Belgium

4 Electrical Engineering Department, Nanoelectronic Center, Technion, 32000 Haifa, Israel;

ababuji@icmab.es

Two derivatives of [1]benzothieno[3,2-b][1]-benzothiophene (BTBT), namely, 2,7-dioctyl-BTBT (C8-BTBT) and 2,7-diphenyl-BTBT (DPh-BTBT), belonging to one of the best performing organic semiconductor (OSC) families, have been employed to investigate the influence of the substitutional side groups on the properties of the interface created when they are in contact with dopant molecules. As a molecular p-dopant, the fluorinated fullerene $C_{60}F_{48}$ is used because of its adequate electronic levels and its bulky molecular structure. Despite the dissimilarity introduced by the OSC film termination, dopant thin films grown on top adopt

the same (111)-oriented FCC crystalline structure in the two cases. However, the early-stage distribution of the dopant on each OSC film surface is dramatically influenced by the group side, leading to distinct host−dopant interfacial morphologies that strongly affect the nanoscale local work function. In this context, Kelvin probe force microscopy and photoelectron emission spectroscopy provide a comprehensive picture of the interfacial electronic properties. The extent of charge transfer and energy level alignment between OSCs and dopants are debated in light of the differences in the ionization potential of the OSC in the films, the interface nanomorphology, and the electronic coupling with the substrate.

C05

Alternative Monolithic Bottom Gate design for Epitaxial Graphene Field Effect Transistor Devices

Sofia Aslanidou[1,2], Alberto García-García[1], Gemma Rius[1] and Philippe Godignon[1]

1 Institute of Microelectronics of Barcelona (IMB-CNM-CSIC)

2 Universitat Autònoma de Barcelona (UAB)

sofia.aslanidou@imb-cnm.csic.es

Silicon Carbide (SiC) is nowadays a widely accepted semiconductor material for industrial applications. The superior intrinsic properties of SiC compared to Si, combined with the ability of growing epitaxial, high-quality graphene on the SiC wafer [1], make it a reliable alternative for electronic applications. Field-effect transistors (FET), radio frequency (RF) power amplifiers, and sensors are some of the applications of Epigraphene on SiC substrates. In this work, we describe the fabrication and characterization of a novel approach on a back gate architecture. The concept behind our project stands in a previous work [2] where the gate was created by high energy nitrogen implantation to form a buried N+ layer below the FET graphene channel. However, the implantation process generates defects in the SiC crystal leading to the detection of a high leakage current. To overcome this issue, we suggest an alternative approach in which the FET device is built on a 4H-SiC, 4◦ off-axis, N+ doped substrate (the back gate) with a 1μm semi-insulating homoepitaxial layer of SiC compensated with vanadium on top (the dielectric layer). As a result, we avoid any defects in the SiC crystal that would be caused by ion implantation, particularly below the FET active areas where epitaxial graphene will be used as channel. Photolithography patterning for the selective implantation with N was performed to form vertical conduction channels for contacting the SiC substrate from the top side. The implant activation was performed by a thermal annealing at 1650◦C assisted with a protective capping layer. The epitaxial graphene film was grown by high temperature Si sublimation method at 1900˚C under an Ar ambient. The graphene channels were defined by E-beam Lithography (EBL) and reactive-ion etching. EBL was also used for the fabrication of electrical contacts, which consist of thin film metal evaporation (Ti+Au) followed by resist lift-off process. Atomic Force Microscopy (AFM), Raman Spectroscopy and Scanning Electron Microscopy (SEM) were performed for the structural

characterization of the devices. Furthermore, the electrical behavior of the bottom gate and the preliminary electrical characteristics of the devices will be presented.

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C06

Dynamic control of octahedra rotation in perovskites by defect engineering

Jiahui Jia[1,2], Xu He[1,3], Arsalan Akhtar[1], Gervasi Herranz[2] and Miguel Pruneda[1]

1 Catalan Institute of Nanoscience and Nanotechnology (ICN2-CSIC

2) Institute of Materials Science of Barcelona (ICMAB-CSIC)

3 Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain, Louvain-la-Neuve, 1348, Belgium.

jiahui.jia@icn2.cat

Engineering oxygen ocatahedra rotation patterns in ABO_3 perovskites is crucial to design functional materials. In this work, we propose a strategy that exploits antisite defects that create local electric dipoles and interact with rotational degrees of freedom. This approach, which relies on substituting an A site with a smaller ion, paves a way to couple dynamically octahedra rotations to external electric fields. Through density functional theory (DFT) calculations we study Al_La antisite defect in rhombohedral $LaAlO_3$ (rLAO) as a prototype to demonstrate this concept. We show that the antisite structure is strongly coupled to the surrounding O atoms and by tuning the orientation of the local dipole created by the defect, the nearby octahedra tilts can be modified. We calculate the energetics of possible switching paths and address the spatial modulation of the local rotational degrees of freedom to the whole lattice. We note that this approach can be extended to substitutional defects in the A-site and are of general application in perovskites. Therefore, our strategy provides a pathway to generate novel functional materials by modulating the properties of a host material through the manipulation of local defect dipoles with electric fields.

C07

3D silicon detectors for Timing Applications

Òscar Ferrer Naval[1], G. Pellegrini[1], N. Moffat[1]

1 Institute of Microelectronics of Barcelona (IMB-CNM-CSIC)

oscar.ferrer@imb-cnm.csic.es

The upcoming upgrade for the LHC, the High Luminosity – LHC, is going to increase the fluence inside the accelerator by an order of magnitude, implying an increase of the amount of radiation that the silicon sensors in the first layers of the experiments will have to be able to withstand. In addition, the increase of fluence will translate to a higher amount of events happening per unit of time, which will require the sensors to be able to tell them apart, implying a good timing performance. This presentation will focus on highlighting 3D silicon detectors, which consist of p-type wafers on which columnar electrodes are etched vertically, which allow for a shorter electrode distance when compared to the planar counterpart. The shorter electrode distance makes them excellent candidates for radiation hard detectors with good timing performance, showing simulations and experimental results that indicate that 3D detectors can have good performance before and after irradiation.

C08

Unveiling of a new reference electrode - the Metallacarboranes

Jewel Ann Maria Xavier[1], Tania Gracia [2], Clara Viñas [1], María Encarnación Lorenzo Abad [2], Francesc Teixidor [1]

1Institut de Ciencia de Materials de Barcelona (ICMAB-CSIC), Campus de la UAB, Bellaterra, Spain.

2 Departamento de Química Analítica y Análisis Instrumental, Universidad Autónoma de Madrid, Madrid, Spain.

jxavier@icmab.es

θ-shaped metallacarboranes such as COSAN, [3,3´Co(1,2-$C_2B_9H_{11}$)2]-, and FESAN, [3,3´Fe(1,2-$C_2B_9H_{11}$)2]-, are polyhedral clusters having two adjacent carbon atoms on the cluster (Cc) with the metal ion sandwiched between the two carborane units. These boron clusters are attractive owing to their advantageous properties such as non-localized negative charge and 3D-aromaticity, ability to form hydrogen, Cc-H···O and dihydrogen, Cc-H···B-H, bonds, water solubility and derivatization capacity similar to organic compounds. Notably, these transition metal centres are redox active making them even more tempting for electrochemical studies. As the redox couples $Co^{3+/2}$+ and $Fe^{3+/2}$+ are highly reversible with a constant formal potential, they are ideal candidates to be employed as reference electrodes in electrochemical studies. In this regard, we have studied the potential advent of these metallacarboranes as reference electrodes by thoroughly investigating their electrochemical

properties through different experiments. As they are soluble in both organic and aqueous solvents, with only changing the counter cation, they are suitable to be used in both the medias. Hence, has the potential to replace the conventional reference systems such as the ferrocene and its derivatives. The experiments range from proving them to have constant formal potential to pH and temperature dependent studies using the efficient and facile technique of cyclic voltammetry. With this study we aim to introduce metallacarboranes as standard reference electrodes to the scientific community.

SESSION D - ENERGY AND ENVIRONMENT

D01

Hybrid 3D-Printing of 8YSZ electrolyte with scaffold for solid oxide cells applications

Maritta Meyrella dos Santos Lira[1], Natalia Kostretsova [1], Alex Morata [1], Marc Torrell [1], Albert Tarancon [1,2]

1 IREC, Catalonia Institute for Energy Research, Jardins de les Dones de Negre 1, 2º, Sant Adrià del Besós, Barcelona, 08930, Spain

2 ICREA, Passeig Lluís Companys 23, 08010, Barcelona

mlira@irec.cat

Electrochemical-based energy devices such as Solid Oxide Cells (SOC) will be necessary to achieve a modern energy scenario that affords the growing energetic demand and ensures environmental sustainability for the next decades. One of the biggest challenges of renewable energy intermittent production is the efficient storage of the generated surplus. One of the considered solutions with a biggest potential is the use of solid oxide electrolysers to produce hydrogen and its subsequently use as a fuel for energy generation in solid oxide fuel cells or other applications. To optimize the performance of SOC devices different parameters has to be optimized: cell architectures, fabrication steps or the catalytic activity of the composite electrodes. One of the most common way to enhance the performance of the electrodes is the use of a ceramic scaffold to be impregnated by a catalytic active phase in order to maximize the number of active sites on the electrodes, so called triple phase boundaries (TPB).The use of additive manufacturing technologies combined with porous ceramic fabrication techniques can help to optimize the microstructures and geometries of the SOC devices magnifying its performance and reliability. In this present work, we aim to fabricate an innovative and complex structure for YSZ electrolytes with dense and porous parts and optimize the fabrication parameters for the stereo-lithography 3D-printing process to obtain enhanced features of the ceramic supports that will be applied for SOC. The YSZ electrolyte with scaffolds with defined porosity will be fabricated for later functionalization by infiltration of the electrodes. The fabrication of this printed 3D structures can be summarized in three main steps. (i) 3D printing, (ii) debinding and (iii) co-sintering. The fabrication of the porous dense porous electrolyte will be created by: generation of porosity by development of new ceramic pastes and tuning of the printing parameters.

D02

Molecular Engineering of Tuning the Ligand Environment of Atomically Disperse Nickel for Efficient Alcohols Electrochemical-Oxidation

Zhifu Liang[1,4], Daochuan Jiang[3], Xiang Wang[4],Mohsen Shakouri[8],Ting Zhang[1],Zhongjun Li[7],Pengyi Tang [2,6],Jordi Llorca[9],Lijia Liu[5],Yupeng Yuan[3],Marc Heggen,Rafal E[6], Dunin-Borkowski[6],Joan R. Morante[4],Andreu Cabot[4,10],Jordi Arbiol[1,10]

1 Catalan Institute of Nanoscience and Nanotechnology (ICN2-CSIC)

2 Shanghai Institute of Microsystem and Information Technology, Chinese Academy of Sciences, Shanghai 200050, China

3 School of Chemistry and Chemical Engineering, Anhui University, Heifei 230601, Anhui Province, China

4 Catalonia Institute for Energy Research – IREC

5 Department of Chemistry, Western University, 1151 Richmond Street, London, ON

6 Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons and Peter Grünberg Institute Forschungszentrum Jülich GmbH 52425 Jülich, Germany

7 School of Physics, Hefei University of Technology, Hefei 230009, P. R China

8 Canadian Light Source, Saskatoon, S7N 0X4, Canada

9 Institute of Energy Technologies, Department of Chemical Engineering and Barcelona, Research Center in Multiscale Science and Engineering, Universitat Politècnica de Catalunya, EEBE, 08019 Barcelona, Catalonia Spain.

10 ICREA

liang.zhifu@icn2.cat

Herein, we demonstrate that tuning the electronic structure of atomically dispersed nickel actives sites through the modification of their edge coordination environment is an excellent strategy to optimize the performance of nickel-based electrocatalysts toward alcohol electrooxidation in alkaline solution. With this aim, we develop a new organic framework with atomically dispersed nickel. The coordination environment of nickel is modified through the addition of carbonyl (C=O) groups to the organic framework as confirmed by X-ray absorption fine spectroscopy (XAFS) and Fourier Transform Infrared Spectroscopy (FTIR). Such nickel-based organic framework, combined with carbon nanotube (namely Ni-2D-O-SA-CNT), exhibits excellent catalytic activity and durability under operating conditions toward the oxidation of methanol (106 mA cm^{-2} at 0.6 V vs Hg/HgO), ethanol (101 mA cm^{-2}) and benzyl alcohol (77 mA cm^{-2}). These outstanding electrocatalytic activities for alcohol electrooxidation are attributed to the introduction of the carbonyl group in the ligand chemical environment, which enhances the adsorption for alcohol, as revealed by density functional theory calculations. Our work not only introduces a new atomically dispersed Ni-based catalyst, but also demonstrates a new strategy for designing and engineering high-performance catalysts through tuning the chemical electronic structure.

D03

Multimaterial 3D Printing of Functional Ceramics for Solid Oxide Cells

Natalia Kostretsova[1], Marc Nuñez [1], Alex Morata [1], Marc Torrell [1], Albert Tarancón [1,2]

1 IREC, Catalonia Institute for Energy Research, Jardins de les Dones de Negre 1, 2º, Sant Adrià del Besós, Barcelona, 08930, Spain

2 ICREA, Passeig Lluís Companys 23, 08010, Barcelona, Spain

nkostretsova@irec.cat

Solid Oxide Cells (SOC) has been identified as one of the main alternatives to be considered for the deployment of the new renewable energy scenario that has to consider large amounts of energy storage capacities. The reversibility of these devices allows two modes of operation, electrolysis and fuel cell. Electrolysis mode will allow to efficiently store the surplus of the renewable energy is form of hydrogen using Solid Oxide Electrolysis Cells (SOEC). Stored hydrogen will be potentially used as a fuel for clean energy generation using the devices as Solid Oxide Fuel Cells(SOFC). Therefore, SOCs are widely considered to be included in new renewable energy networks due to their high efficiency and capacities. However, SOC geometries and production process are, currently, constrained by the application of various traditional ceramic manufacturing technologies and numerous thermal treatments that makes their production process expensive and time-consuming. The development of ceramic 3D printing technologies represents a high degree of design freedom for the ceramic processing, overcoming the classic limits of the ceramic manufacturing. In this regard, the application of ceramic 3D printing can positively change the SOC manufacturing process in terms of productivity, cost, rate, and reliability while allows a more flexible production. Thus, the use of hybrid ceramic 3D printing technologies makes possible the fabrication of self-supported complete SOC devices during one-step printing. For this purpose, hybrid 3D printing technology based on stereolithography (SLA) and robocasting (RC) has been developed. The technique allows to fabricate a single part with a combination of several different functional ceramic materials. The self-supported SOC is based on 8YSZ that is also used as the electrolyte and fabricated by SLA, while state-of-the-art SOC electrode materials are deposited by RC. Fully 3D printed SOC cells, their co-sintering process, and characterization are presented in this work, while advantages, limitations, and perspectives of the manufacturing process are discussed.

D04

Efficient chemical doping of organic field effect transistors using an aqueous iodine solution

Jinghai Li[1], Raphael Pfattner [1], Marta Mas-Torrent [1]

1Institut de Ciencia de Materials de Barcelona (ICMAB-CSIC)

jinghaili@icmab.es

Organic semiconductor films fabricated from solution processes have great potential for spurring the development of electronic devices. However, the performance of such devices is affected by external factors such as contact resistance. Here, thin films of the organic semiconductor C8-BTBT-C8 blended with polystyrene (PS)were prepared by bar-assisted meniscus shearing (BAMs) technique using a home-designed equipment. All the fabrication process was carried out under ambient conditions. This film has shown high crystalline film but with worse electrical properties because of the high contact resistance and high injection barrier. Iodine water solution was used as dopant material introduced in the semiconductor, and the devices after doped showed much lower contact resistance and ideal electrical properties.

D05

Quasi-double-star nickel and iron active sites for high-efficiency carbon dioxide electroreduction

Xu Han[1], Ting Zhang[1,2], Jordi Arbiol[1,3]

1 Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Campus UAB, Bellaterra, Barcelona, 08193, Catalonia, Spain

2 Catalonia Institute for Energy Research (IREC), Jardins de les Dones de Negre 1, Sant Adrià del Besòs, Barcelona, 08930, Catalonia, Spain

3 ICREA, Pg. Lluís Companys 23, Barcelona, 08010, Catalonia, Spain

xu.han@icn2.cat

Although the Faradaic efficiencies (FEs) obtained on most of the Ni based single-atom catalysts (Ni-N-C) are satisfactory (generally > 90 %) for electrochemical transfer CO_2 to CO, the practical application is still limited by their high overpotentials (> 600 mV vs. RHE), which implies a higher consumption of energy to drive the CO_2 RR.[1] In this work, we have prepared a quasi-double star catalyst composed of nearby Ni and Fe active sites through a simple pyrolysis of Ni and Fe co-doped Zn-based MOFs in order to achieve a high selectivity at a low overpotential during CO_2 RR. Due to the different Z contrast among Ni, Fe, N, O and C elements, the obtained Ni/Fe-N-C catalyst has been directly characterized by AC-HAADF

STEM, showing the homogenously dispersed spots in the substrate, which confirms that Ni and Fe are atomically dispersed in the Ni/Fe-N-C sample, which is accordance with the XAS results. Benefiting from the nearby Ni and Fe active sites, the optimized Ni/Fe-N-C catalyst shows an exclusive selectivity (a maximum FE (CO) of 98 %) at a low overpotential of 390 mV vs. RHE, which is superior to both single metal counterparts (Ni-N-C and Fe-N-C catalysts) and other state-of-the-art M-N-C catalysts, which is further supported by DFT results.

[1] T. Zhang, X. Han, H. Liu, M. Biset-Peiró, X. Zhang, P. Tan, P. Tang, B. Yang, L. Zheng, J. R. Morante, J. Arbiol, *Energy Environ. Sci.* **2021**, *14*, 4847-4857.

PLENARY TALK

Dr. Montse Pont

ALBA Synchrotron



Dr. Montse Pont is coordinator of operating activities at the ALBA Synchrotron and a member of the management board. She earned her PhD in Physics in 1990 at Universitat Autònoma de Barcelona and KTH Royal Institute of Technology in Stockholm.

She received one of the first postdoctoral fellowships for the design of the Spanish synchrotron light source in 1994. Before the formal approval of that project, she moved to Karlsruhe, in Germany, to participate in the design and construction of the ANKA light source. In 2004 she moved back to Barcelona to join the ALBA Synchrotron. She has been the head of accelerator operations during eight years and last year she joined the ALBA management as coordinator of the operating activities.

ALBA II, the upgrade project of the ALBA Synchrotron

ALBA is a 3.0 GeV third generation synchrotron light source that started operation in 2012 with 7 beamlines. Today, ALBA is operating 8 beamlines, there are 2 under commissioning and 3 additional ones under construction. With 5000h of operation per year, ALBA serves a consolidated user community and it is well established in its field. Now it is the right time to consider the long-term future of ALBA. Latest developments in the field of the so-called Diffraction Limited Storage Rings offer the opportunity to exploit much brighter photon beams and an increased coherence over a large energy range. The gains will offer important new scientific opportunities in a wide range of science of particular importance to address the challenges of our society. In the talk after reviewing the milestones of ALBA, the upgrade project ALBA II will be presented.

PLENARY TALK

Prof. César de la Fuente



University of Pennsylvania

César de la Fuente is a Presidential Assistant Professor at the University of Pennsylvania, where he leads the Machine Biology Group whose goal is to combine the power of machines and biology to understand, prevent, and treat infectious diseases. Specifically, he pioneered the development of the first antibiotic designed by a computer with efficacy in animals, designed algorithms for antibiotic discovery, reprogrammed venoms into antimicrobials, created novel resistance-proof antimicrobial materials, and invented rapid low-cost diagnostics for COVID-19 and other infections.

De la Fuente is an NIH MIRA investigator and has received recognition and research funding from numerous other groups. Prof. de la Fuente has received over 50 awards. He was recognized by MIT Technology Review as one of the world's top innovators for "digitizing evolution to make better antibiotics". He was selected as the inaugural recipient of the Langer Prize, an ACS Kavli Emerging Leader in Chemistry, and received the AIChE's 35 Under 35 Award and the ACS Infectious Diseases Young Investigator Award. In 2021, he received the Thermo Fisher Award, and the EMBS Academic Early Career Achievement Award "For the pioneering development of novel antibiotics designed using principles from computation, engineering, and biology." Most recently, Prof. de la Fuente was awarded the prestigious Princess of Girona Prize for Scientific Research. Prof. de la Fuente has given over 150 invited lectures and his scientific discoveries have yielded around 100 publications, including papers in Nature Biomedical Engineering, Nature Communications, PNAS, ACS Nano, Cell, Nature Chemical Biology, Advanced Materials, and multiple patents.

Machine Biology for Infectious Diseases

Machines have the potential to outperform humans and revolutionize our world. In this talk, I will describe our efforts using machines to develop computational approaches for antibiotic discovery, as well as low-cost rapid diagnostics. Computers can already be programmed for superhuman pattern recognition of images and text. In order for machines to discover novel antibiotics, they have to first be trained to sort through the many characteristics of molecules and determine which properties should be retained, suppressed, or enhanced to optimize antimicrobial activity. Said differently, machines need to be able to understand, read, write, and eventually create new molecules. I will discuss how we trained a computer to execute a fitness function following a Darwinian algorithm of evolution to select for molecular structures that interact with bacterial membranes, yielding the first artificial antimicrobials that kill bacteria both in vitro and in relevant animal models. My lab has also developed pattern recognition

algorithms to mine the human proteome, identifying throughout the body thousands of antibiotics encoded in proteins with unrelated biological function, and has applied computational tools to successfully reprogram venoms into novel antimicrobials. I will also describe the development of low-cost diagnostic biosensors for COVID-19, further substantiating the exciting potential of machine biology. Computer-generated designs and innovations at the intersection between machines and biology may help to replenish our arsenal of effective drugs and generate novel diagnostics, providing much-needed solutions to global health problems caused by infectious diseases.

WORKSHOP 1

Dr.Salvador Ferré Benedicto



Eduscopi/ Universitat de Vic (UVic)

Salvador Ferré obtained his PhD in Biochemistry and Molecular Biology in 2007 at Universitat de Barcelona. He continued his scientific career in the communication arena by starting a blog that would eventually lead him to write and edit outreach books and digital textbooks. A few years ago he co-founded Eduscopi. At the present, except for directing Eduscopi he is coordinating the Postgraduate Studies in Scientific Communication of Universitat de Vic (UVic) in Barcelona.

His excellent career and extensive experience has been reflected in the publication of many digital or paper books, including 8 related with scientific divulgation, more than 25 textbooks and 1 poem book, working as author, editor or coordinator. In addition, he writes scripts, records videos and podcasts, conducts trainings and, above all, tries to transmit the passion for science by all possible means.

Scientific Communication

"So, what exactly is your research about?..." More than just an uncomfortable question you might get from a relative, explaining your science to a non-expert audience is an increasingly important skill for our impact as researchers, and can even be key for getting and implementing funded projects. The goal of this talk is share with you tools and concepts to adapt the messages to reach different and broader audiences.

WORKSHOP 2

Dr. Xavier Borrisé



IMB-CNM-CSIC

Dr. Xavier Borrisé is in charge of the Nanolithography Laboratory at the Clean-Room of the IMB-CNM-CSIC.

Dr. Borrisé graduated in Physics and later gained a Ph.D in Electronics Engineering from the Universitat Autònoma of Barcelona. After 5 years as a Ramon y Cajal Researcher at the IMB-CNM-CSIC in the group of Nanofabrication headed by Francesc Pérez-Murano, he joined the ICN in 2007 in order to start up the nanolithography facilities within the CNM clean-room.

His main research activites and achievements are in the Top-Down approximation to Nanothecnology, Nanofabrication and Nanolithography with over 60 publications. Dr. Borrisé developed the first SNOM in Spain during his Ph.D, he is working since many years on the development of nanomechanical devices for mass sensing by using different nanolithography techniques (EBL, NIL, FIB). He is also working in developing nanolitho techniques for nanolectrodes and sensors devoted to different sensing areas as DNA sensing or protein detection.

Mr.Albert Guerrero



IMB-CNM-CSIC

Albert Guerrero is one of the engineers of the Nanolithography Laboratory at the Clean-Room of the IMB-CNM-CSIC. Albert graduated in Nanoscience and Nanotechnology at the Universitat Autònoma de Barcelona. During his last year, he did external practices at the Electronic Microscopy Unit lead by Dr. Belén Ballesteros at ICN2. Also, he obtained his MSc in Advanced Nanoscience and Nanotechnology in the same university, with a master's thesis devoted to the fabrication of plasmonic nanostructures for LiDAR applications.

He joined IMB-CNM-CSIC through a grant of the Spanish Ministerio de Economía y Empresa (MINECO) starting to work at the IMB-CNM-CSIC Nanolithography Laboratory on 2016 where he has worked with different characterization and fabrication techniques such as SEM, AFM, EBL and, recently, LL.

Into the Nanolaboratory!

"I need to measure the layer structure of my sample, but how? Which materials are there before and after this experiment? I would like to prepare this device, how can I do it? These, and other questions are usual among the students and scientists while they develop their ideas. In this workshop it will be explained which techniques can be used to prepare and to characterize different samples using several systems. So come with me to the nanolaboratory!"

ROUND TABLE – DIVERSITY IN STEM DISCIPLINES

Dr. Clara Barker



Centre for Applied Superconductivity at Oxford

Dr Clara Barker (https://www.cfas.ox.ac.uk/clara) is a thin film Material Scientist who manages the Centre for Applied Superconductivity at Oxford. Clara is the chair of the LGBT+ advisory group at Oxford University, Dean for equality and diversity at Linacre College and in 2018 she won the first diversity role model award from the University. She is also a member of the both the Royal Society and the Girls School Alliance E&D committees. In her spare time, she runs a youth group for LGBTI+ people, with a support group for their parents. She is the recipient of the Points of Light Award from the UK Prime Minister in 2018, has written for various publications, delivered many talks on LGBTI+ issues and diversity in academia, including a TEDx talk in 2018, (https://youtu.be/cReiIVsgNGs) and was highlighted in Nature in early 2021 https://www.nature.com/articles/d41586-021-00024-z .

Dr. Carmen Botella



School of Engineering of the Universitat de València

Dr. Carmen Botella Mascarell is an associate professor in the school of engineering of the Universitat de València. She received the telecommunication engineering degree and the Ph.D. degree from the Universitat Politècnica de València, Spain, in 2003 and 2008, respectively. After that she carried out her postdoctoral research in the Chalmers University of Technology (Gothenburg, Sweden), where she was involved in several national and European research projects targeting 4G and beyond mobile communications (WINNER+ and ARTIST4G among others). Her research interests include the general areas of coordination and cooperation for future 5G and beyond systems. Apart from that, she has done research on gender diversity in ICT-STEM disciplines and published several articles on this topic.

Prof. Xavier Roque



Universitat Autonoma de Barcelona (UAB)

Xavier Roqué is professor of History of Science at the Autonomous University of Barcelona (UAB) and a member of the Department of Philosophy and the Institute of History of Science (IHC). After graduating from the Physics Department, he received his doctorate in History of Science (UAB, 1993) and carried out postdoctoral stays in Cambridge and Paris. He has been a visiting professor at the universities of Cambridge (2011) and Uppsala (2013).

His research and publications focus on contemporary physics and the relationship between science, culture and gender. Recent publications include De la Guerra Fría al calentamiento global. Estados Unidos, España y el nuevo orden científico mundial (Libros de la Catarata, 2018, edited with L. Camprubí and F. Sáez de Adana); Albert Einstein. La relativitat a l'abast de tothom (translated and annotated by X. Roqué, Obrador Edèndum, 2018); and "The cultural significance of physics and evolution in Francoist Spain" (with Clara Florensa), Culture & History Digital Journal 10 (2021): 1–14. He is currently IP of the research project "Small science: a historical survey of contemporary small-scale research (SMALLSCIENCE, PID2019-105131GB-I00)" and coordinator of the new degree on Science, Technology and Humanities (UAB-UAM-UC3M).

Prof. Gemma Garcia



Universitat Autonoma de Barcelona (UAB) / AMIT-Cat

Gemma Garcia Alonso is a professor in the Department of Physics and Dean of faculty of science at the Autonomous University of Barcelona (UAB). She did her bachelor's degree in Physics from the Paul Sabatier University in Toulouse and master's degree in Material Science from the National Polytechnic Institute of Toulouse. After that she obtained her doctorate in Physical Sciences from the University of Barcelona. She was a contracted researcher at the Barcelona Institute of Materials Science (ICMAB-CSIC) from 1999 to 2004, and then she joined the Department of Physics, UAB. She has been the coordinator of the second cycle in Materials Engineering, associate coordinator of the Degree in Nanoscience and Nanotechnology, Vice-Dean of Students and Promotion, and Vice-Dean of Undergraduate Academic Affairs at UAB. Her main research focuses on the development of thin film materials for energy applications (fuel cells, hydrogen storage, thermoelectric).

Prof. Gemma Garcia is a member of the AMIT-Cat (Association of Women Researchers and Technologists, Catalonia node) association and has actively participated in AMIT-Cat activities, particularly in 2018 in the STEM amb tu project. She is also the representative of gender politics at the Faculty of Science, UAB.

POSTER SESSION

P01

Organ-on-a-chip device with integrated semitransparent organic electrodes for barrier function monitoring

Denise Marrero[1,2,3], Xavi Illa[1,2], Mar Alvarez[1,2], and Rosa Villa[1,2]

1 Institute of Microelectronics of Barcelona (IMB-CNM-CSIC)

2 Universidad Autónoma de Barcelona (UAB), Bellaterra, 08193, Barcelona, Spain

3 Centro de Investigación Biomédica en Red en Bioingeniería, Biomateriales y Nanomedicina (CIBER-BBN), Madrid, 50018, Spain

denise.marrero@imb-cnm.csic.es

Biological barriers have intrinsic electrical properties that yield information about cellular barrier function and integrity. Monitoring such properties is of paramount importance to study and develop relevant Organ-on-a-Chip (OoC) models. However, large data discrepancies exist between different models due to a lack of standardization in impedance-based OoC design and complex data analysis. In this work, we have developed an OoC platform with integrated poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) electrodes to perform electrochemical impedance spectroscopy on cellular barriers. The electrodes fully meet the requirements of OoC applications of good biocompatibility, high electrode transmittance, planar impedance response over a large frequency range (10-105 Hz), and low cutoff frequency. Additionally, the device is reusable except for the cell culture membrane, which reduces the cost and environmental impact.

P02

Piezoelectric ZnO nanostructures integrated in microdevices for cell stimulation

Laura Lefaix Fernández[1], Andreu Blanquer[2], Lucie Bacakova[2], **Gonzalo Murillo**[1]

1 Instituto de Microelectrónica de Barcelona (IMB-CNM, CSIC), Barcelona, Spain

2 Institute of Physiology of the Czech Academy of Sciences, Prague, Czech Republic

gonzalo.murillo@csic.es

The ability of cells to respond to electrical stimuli by proliferating, differentiating and migrating has largely been proved. Also, other specific electrical signals such as the nerve impulse and muscle contraction happen in neurons and muscle cells due to electrical processes. The use of electrical devices to improve these electrical properties of the cell and thus establish a way

of communication between the electrical signal delivered and the final stimulus produced has gradually increased in the field of bioelectronic medicine through the years. To safely deliver the electrical signal without the need of cables or electromagnetic waves that can alter the cells and their environment, the use of piezoelectric materials is being implemented for this kind of applications, as they generate an electric dipole between their surfaces, when mechanically stressed. Ultrasounds, in the biomedical range (MHz), can be used to actuate the piezoelectric materials and as a way of communication with the microdevices from outside of our body. In this work, we have developed, through microfabrication techniques and chemical synthesis, a microdevice with piezoelectric nanostructures capable of stimulating a single cell. These microparticles are defined by cleanroom processing and used as templates to grow zinc oxide nanosheets (ZnO NSs) on their surface. Then, they are peeled off and suspended in a biocompatible liquid ready to be added to a cell culture. In our previous works, ZnO NSs have been tested as substrate for Saos-2 cell cultures, demonstrating that the electromechanical interaction between the cells and the NSs can electrically stimulate the voltage-controlled calcium channels (VGCCs) present in the membrane, increasing spontaneously the calcium concentration in the cell cytoplasm. In addition, our microdevices have been proved cytocompatible and a study to know the internalization and the positioning with respect to the cells has been carried out. The electrical field generated by the NSs in contact with the cell membrane seems to be enough to trigger the opening of VGCCs, according to our finite element modelling (FEM). We are currently performing new biological experiments using ultrasonic pulses to stimulate the microdevices and study the calcium peak pattern produced by the activated cells. These remotely actuated microdevices to electromodulate cell membrane potential have impactful applications in electroceuticals and bioelectronic medicines.

P03

Resonant microelectromechanical systems for bioelectronic microdevices and electroceuticals

Marc Navarro Pons[1], Laura Llefaix[1]

1 Institute of Microelectronics of Barcelona (IMB-CNM-CSIC)

marc.navarro@imb-cnm.csic.es

Electrical cell stimulation is capable of triggering electrical cell signals that are key in regulating cell processes as proliferation, migration, differentiation, orientation and apoptosis. Moreover, other specific electrical signals happen in excitable cells such as neurons and muscle cells. Because of that, electrical cell stimulation is used in regenerative medicine and the therapeutically research of immunological illness with the usage of Electroceuticals. Electrostimulation can be achieved by directly applying an electric field using electrodes or indirectly, by inducing an electric field from a generated magnetic field or using piezoelectric materials, who accumulate charge in response to applied mechanical stress because a rearrangement of its ions in their crystalline structure. Ultrasounds can be used to transmit mechanical stress to a piezoelectric material deep into biological tissues, and are used as a

way to power piezoelectric microelectromechanical systems (PiezoMEMS) in the field of biomedicine and biomedical engineering. In our project, we are focused on design, model, and optimize a variety of resonant piezoMEMS using Finite Element Modelling (FEM) software COMSOL Multiphysics and develop them afterwards through microfabrication techniques in a clean room process. The devices enable cell stimulation and are powered using energy harvesting from ultrasound signals within biomedical range (1-20 MHz). The designed piezoMEMS have a size similar to a cell, of around 80 µm of diameter and enable local cell electrostimulation. Through COMSOL simulation, the devices present a quality factor similar to the state of the art underwater resonant devices, their power output and electrical field generated when stimulated using a 0.1 MPa ultrasonic wave are ~40 µW and ~100 mV, which, according to bibliography, are sufficient according to bibliography to electrically stimulate cells. The following steps in a near future are to finish the microfabrication processes and validate the simulation data through studying the opening of Voltage Calcium Channels (VGCCs) in a variety of cells when stimulated using ultrasonic pulses.

P04

Electrolyte-Gated Filed-Effect Transistors for sensing an Alzheimer's disease biomarker

S. Ruiz-Molina[1], S. Ricci[2], S. Casalini[2], M. Mas-Torrent[1],

1 Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus UAB, 08193 Bellaterra, Spain

2 Università degli studi di Padova, departamento di scienze chimiche, via francesco Marzolo 1, 35131, Padova, Italy

sruiz@icmab.es

Electrolyte-Gated Organic Field-Effect Transistors (EGOFETs) have been investigated recently as a useful means for biological sensing. Their working principle is based on converting a chemical event into a readable electrical signal. These devices can be prepared at low cost and on flexible substrates and present high sensitivity and specificity. In this work, we report the study of Aβ1-40 peptide aggregation kinetics using a label-free EGOFET immunosensor. Amyloid-beta 1-40 is a peptide present in the brain of Alzheimer's disease (AD) patients. It tends to aggregate in oligomers, which are believed as major toxic effects in this pathology. Thus, they are considered promising biomarkers for its diagnosis and therapy. The sensing element of EGOFETs resides at the Au gate-electrolyte interface. One strategy of Au surface engineering with antibodies has been developed. The validation of this protocol has been carried out using electrochemistry, employing Cyclic Voltammetry (C.V.) and Electrochemical Impedance Spectroscopy (E.I.S.) as characterization techniques. In the same way, the aggregation process has been characterized by EGOFET transfer characteristics, using PBS 1X as electrolyte. The results show that the maximum oligomer species are found after 2 hours of incubation in both electrochemical and EGOFET characterization. The final purpose is to combine the EGOFET with a microfluidic system paving the way towards the fabrication of simple and cost-effective devices that allows continuous measurements and more efficient diagnosis.

P05

Electrothermal modeling of Mo/Au Transition-Edge Sensors

Manel Mas Martín[1], Carlos Pobes[2], Agustín Camón[2], Juan Bolea[3], Pavel Strichovanec[2], Lourdes Fàbrega [1]

1Institut de Ciencia de Materials de Barcelona (ICMAB-CSIC)

2 Instituto de Nanociencia y Materiales de Aragón (INMA)

3 Centro Universitario de la Defensa, Zaragoza

mmas2@icmab.es

The fundamental parameters of Transition-Edge Sensors (TESs) are typically extracted from measurements of the I-V curves and complex impedance Z(w). For this extraction, an electrothermal model is required, that is, a description of the number of thermal blocks constituting the devices and their configuration. The simplest, most widely used method assumes a single thermal block. While this approximation may seem quite reasonable especially for TESs without absorber, the shape of the Z(w) in bare TESs for some operation conditions clearly reveals that the single thermal block model does not properly describe the data; therefore, by using it some errors in the estimates of TES parameters could exist. We have measured the complex impedance of bare Mo/Au TES, that is, sensors without absorber, as a function of bias and size (for a given bath temperature). We show that a two-thermal block model describes the observed Z(w) much better than a single thermal block. Finally, we analyze the impact on the extracted TES parameters of the different block configurations and hypotheses that can be used to perform the fittings.

P06

Tailored Spin-Textures in Hybrid Superconducting-Ferromagnetic Structures

Aleix Barrera Català[1], Jordi Alcalà[1], Anna Palau[1]

1Institut de Ciencia de Materials de Barcelona (ICMAB-CSIC)

abarrera@icmab.es

In the last decade, the information processing has been a focus of interest for its potential applications in many fields of the society. Nowadays, there are a lot of systems able to storage and process information in a fast way. However, the desire of apply the Internet of Things in all possible objects and places, requires the development of new processing technologies that work in nano and micro scale in an efficient and sustainable way. Regarding to this field, multifunctional oxides have attracted special attention for their capacity to modify their

magnetic or electric properties by applying an adequate stimulus. In specific, superconducting cuprates mixed with ferromagnetic materials (FM-SC hybrids) have presented novel and unique magnetic tunability. Here, we show that by combining YBCO (SC) and permalloy (FM) materials in hybrid devices, one can manipulate magnetic textures, through loss-less superconducting stray fields or transport super-currents. Multiple magnetic states with different magnetoresistance signal can be stabilized at remanence and modified by applying small magnetic fields or currents. The proposed approach opens new venues for energy-efficient information storage and manipulation.

P07

Determination of Chemical Oxygen Demand (COD) Using Nanoparticle-Modified Voltammetric Sensors and Electronic Tongue Principles

Qing Wang[1], Manel del Valle[1]

1 Universitat Autònoma de Barcelona (UAB)

qing.wang2@e-campus.uab.cat

Chemical Oxygen Demand (COD) is a widely used parameter in analysing and controlling the degree of pollution in water. COD is defined as the amount of molecular oxygen (in milligrams of O_2) required to decompose all the organic compounds in 1 L of aqueous solution to carbon dioxide and water. There are many methods reported for COD determination, such as the conventional dichromate titration method. Electro-oxidizing the organic contaminants to completely transform them into CO_2 and H_2O using sensors is considered the best method for COD estimation. Increasing attention has been paid to electrochemical methods because they are highly sensitive, time-saving, low-cost, and easy to operate. In this sense, copper electrodes have been reported based on the fact that copper in alkaline media acts as a powerful electrocatalyst for oxidation of aminoacids and carbohydrates, which are believed to be the major culprits for organic pollution. Cyclic voltammetry was the technique used to obtain the voltammetric responses. Commonly, different organic compounds show different shapes of cyclic voltammograms and different current intensity in different concentrations. In this work, four kinds of electrodes modified with copper (Cu)/copper oxide (CuO)/nickel copper alloy (Ni Cu alloy) nanoparticles were studied for COD analysis employing the cyclic voltammetry technique: Nafion film covered electrodeposited CuO/Cu nanoparticle electrode (E1), Cu nanoparticle-graphite composite electrode (E2), CuO nanoparticle-graphite composite electrode (E3) and Ni Cu alloy nanoparticle-graphite composite electrode (E4). The COD values were determined by the ploted calibration of COD values vs. the current intensity. Glucose, glycine, potassium hydrogen phthalate (KHP) and ethylene glycol, which show different reducibilities, were chosen to be the standard substances to play the role of organic contaminants with different degradation difficulties. From the obtained cyclic voltammograms, we can see that glucose is very easy to be oxidized by those four electrodes and electrode E1 shows the best performance, with a linear range of 19.2~1120.8 mg/L and limit of detection of 27.5 mg/L (calculated based on the formula $3\sigma/k$). Besides, the compound KHP is very difficult to be oxidized by these four electrodes. Nevertheless, the obtained voltammetric profiles

presented different shapes with the tested organic compounds, suggesting these four electrodes can compose an electronic tongue array for multivariate analysis. As a result, the main component of river samples, which is easy or difficult to be degraded, can be evaluated by the PCA technique. This evaluation is very helpful for the accuracy of COD detection. The resulting sensor-based method demonstrates great potential not only for estimating the precise value of COD, but for predicting the difficulty behavior in its degradation, in a simple, fast, and clean methodology, which is completely suited to the present demands of green techniques.

P08

Tuning the electronic structure of High Temperature Superconducting films by field-induced oxygen diffusion

J. Alcalà[1], A. Fernández-Rodríguez[1], S. Marinkovic[2], S. Collienne[2], S. Blanco Alvarez[2], S. Melinte[2], X. Granados[1], N. Mestres[1], A. V. Silhanek[2], A. Palau[1]

1Institut de Ciencia de Materials de Barcelona (ICMAB-CSIC)

2 Experimental Physics of Nanostructured Materials, Q-MAT, CESAM, Université de Lieġe, B-4000 Lieġe, Belgium

jalcala@icmab.es

Modulation of carrier concentration in strongly correlated oxides offers the unique opportunity to induce different phases in the same material, which dramatically change their physical properties. Specially, the possibility to reversibly modify the metal-insulator transition (MIT) in perovskite oxides, by means of an electric field, as the external control parameter [1], is a very active area of research in condensed matter physics, and a promising technique to generate new solid-state devices with exciting functionalities. In this contribution we will show the electric manipulation of the superconducting to insulator phase transition (SIT) in high temperature superconductor $YBa_2Cu_3O_7$-films by field-induced oxygen doping [2]. Temperature-dependent transport and resistance measurements, together with micro-Raman experiments were performed to evaluate the local oxygen diffusion through the material in different electrode configurations. In particular, the implication of the intrinsic anisotropic oxygen diffusion in cuprates has been studied experimentally and corroborated with simulation. We demonstrate that non-volatile volume phase transitions can be locally modulated to generate transistor-like devices, with free-resistance channels, in which the electric field magnitude and direction, temperature, and anisotropic oxygen mobility determine their characteristics.

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P09

High throughput fabrication of a Single Electron Devices based on Silicon Nanowires with embedded Quantum Dot

D. Bricio-Blázquez[1], A. Kapas[1,2], A. Guerrero[1], J. Sánchez[1], A. García[1], R. Mas[1], X. Borrisé[3], J. Bausells[1], F. Perez-Murano[1] and J. Llobet[1]

[1]Institute of Microelectronics of Barcelona (IMB-CNM CSIC), Bellaterra, Catalonia, E-08193, Spain

[2]Universitat Autónoma de Barcelona (UAB), Bellaterra, Catalonia, E-08193, Spain

[3]Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and The BIST, Bellaterra, 08193, Catalonia, Spain

David.Bricio@imb-cnm.csic.es

The purpose of this work is to design an approach for the high throughput fabrication of Single Electron Devices (SED). The Source and the Drain terminals of such devices, will be connected by a Silicon Nanowire (SiNW). An implanted Quantum Dot (QD) will be embedded in the SiNW to operate as an electrical island. The approach is based on 5 lithographic levels, it employs a Mix-And-Match strategy combining optical and Electron Beam Lithography, and it includes the development of implantation and thermal processes to place a QD in the chosen position.

P10

Magnetic response on bending strain of epitaxial spinel and epsilon iron oxide thin films on flexible Mica substrates

Darla Mare[1], Zheng Ma[1,3], Vassil Skumryev[2,3], Florencio Sánchez[1], Nico Dix[1], Marti Gich[1]

1 Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus UAB, Bellaterra 08193, Barcelona, Spain

2 Institució Catalana de Recerca i Estudis Avançats (ICREA), Barcelona 08010, Spain

3 Universitat Autònoma de Barcelona, Departament de Física, Bellaterra 08193, Spain

dmare@icmab.es

We present our study on strain-controlled magnetic properties of functional iron oxide thin films grown on flexible mica substrates. This unique system allows a simple approach to probe the effect of lattice deformation, by bending the substrate, on the magnetic anisotropy of epitaxial thin films. We prepared a series of common spinel ferrite (XFe_2O_4 [X = Fe,Ni,Co]) and complex ε-Fe_2O_3 thin films as test system due to their distinct intrinsic magnetocrystalline anisotropy. We present a detailed study probing the effect of tensile to compressive bending strain on magnetic properties at room temperature. Furthermore, we probe the low temperature transitions of magnetite and epsilon iron oxide by MT cycles and MH hysteresis loops at varied T. Magnetite Fe_3O_4 thin films show a clear dependence on different bending

strains displaying changes in the coercive field, remnant/saturation magnetization and Verwey transition. In contrast the $NiFe_2O_4$, $CoFe_2O_4$ and ε-Fe_2O_3 thin film only show weak or no significant variation of magnetic properties with strain although reported otherwise in literature. We discuss these reported results with respect to our samples.

P11

Patterning Bacterial Cellulose Films with Iron Oxide Nanoparticles and Magnetic Resonance Imaging Monitoring

Meslier Thomas[1], Mira-Cuenca Cristina[1], Roig-Sanchez Soledad[1], Laromaine Anna[1], Roig Anna[1]

1 Institute of Materials Science of Barcelona, Campus UAB, Bellaterra, Catalonia, 08193, Spain

tmeslier@icmab.es

Biomaterials derived from nature can offer sustainable, biomimetic, and bio interactive solutions. Bacterial cellulose (BC) is a natural biopolymer gaining popularity in the medical field due to its biocompatibility, excellent mechanical properties, and animal-free origin. Those attributes, together with its optimal conformability to different surfaces and high water holding capacity, have endorsed the use of BC films in wound healing, tissue engineering, implants, or wearable sensors. The functionalization of the BC films with nanoparticles (NPs) and the spatial control of their disposition in a BC substrate could further boost BC opportunities in those sectors. Here we report on an original method to deposit superparamagnetic iron oxide NPs in selected areas of a flat BC film using a screen-printing process to create ad hoc NPs patterns on the film surface.

P12

A morphological and structural investigation on the growth of C8O-BTBT-OC8 thin films

Shunya Yan[1], Adara Babuji[2], Francesco Silvestri[2], **Ocal Carmen***, **Esther Barrena***,

1Institut de Ciencia de Materials de Barcelona (ICMAB-CSIC)

syan@icmab.es

In this work we have chosen 2,7-bis(octyloxy) [1]benzothieno[3,2-b]-benzothiophene (C8O-BTBT-OC8) as organic semiconductor because it belongs to a family of derivatives of BTBT (benzothieno[3,2-b]-benzothiophene) with good electrical performance in thin films organic field effect transistors. It has been reported that thin films C8O-BTBT-OC8 exhibit a substrate-induced structure that differs from the bulk form and a temperature-induced polymorphism that may have important implications for the electrical performance in OFETs. In this work we present a morphological and structural investigation on the growth of C8O-BTBT-OC8 on

silicon dioxide for different thicknesses, with a particular focus on the effect of the substrate temperature, during growth and after a post-annealing treatment.

P13

Acrylate segment effect in Polyurethane-Acrylate hybrids. Synthesis and applications

Guillem Romero-Sabat[1], S. Medel, PhD[1], L. Granda, PhD[1], F. Fenollosa-Artes[2]

1 Leitat Technological Center, Carrer de la Innovació, 2 (Terrassa, Spain)

2 Centre CIM, Universitat Politècnica de Catalunya (CIM UPC), Carrer de Llorens i Artigas, 12 (Barcelona, Spain)

gromero@leitat.org

Thanks to their versatility, Polyurethane-Acrylate hybrid polymers can find its way through a wide range of applications where a specialty polymer is needed. Moreover, with a deep understanding about how each building block affects the overall polymer behavior, we can potentially synthesize a tunned material for every single use. With that objective in mind, a series of UV-curable isophorone diisocyanate-based poly(ether-urethane)methacrylate were synthesized by a two-step polymerization process. Modifications in the soft/hard segment ratio (65:35, 80:20) as well as in the acrylate monomer(HEMA, HPMA & PEGMA 360) and concentration (2.5, 5, 7.5 w.t.%) of acrylic segment were introduced during the synthesis and their effects on the overal physicochemical properties were investigated. The coherency obtained in the results allow for a successful prediction of the material's behavior depending on the monomer selection during the synthesis process. Particularly, these findings can provide an ease in the production of personalized soft tissue surgical guides manufactured by 3D printing techniques.

P14

Copper oxide nanocubes wrapping metals by microwave synthesis

Miquel Torras[1], Anna Roig[1]

1Institut de Ciencia de Materials de Barcelona (ICMAB-CSIC)

mtorras@icmab.es

Copper (I) oxide (Cu2O, cuprite) is one of the most interesting copper oxide phases for photocatalysis. However, fast recombination and stability remain an obstacle, as Cu2O can be easily oxidized or reduced by the photogenerated carriers. By doping Cu2O with ions or combining it with metal or semiconductor nanoparticles (NPs), higher photocatalytic activities have been achieved. Here we report for the first time on noble metal-Cu2O heterostructures

using a microwave-assisted synthesis. Microwave-assisted chemistry is becoming attractive in all areas of synthetic chemistry; it is fast, efficient in terms of energy consumption and environmentally friendly. Microwave-synthetic routes are also gaining importance in colloidal chemistry, including the fabrication of multimaterial or metastable alloy nanoparticles. I will report on a universal microwave-assisted two-step synthesis to fabricate noble metals [Au, Ag, Pd, Pt]/Cu_2O heterostructures in a short time. By using Au, Ag or Pd, nanoparticles as seeds, the final material consist of Cu_2O nanocubes wrapping those metal particles. This was achieved by benefiting from the MW selective heating, the metal nanoparticles in the reaction media act as a nucleation sites for the Cu_2O to grow. Interestingly, no size refining step was introduced before size analysis of the obtained monodispersed nanocubes. Moreover, the reproducibility and scalability of the process could be demonstrated. Furthermore, we have proposed the synthetic parameters that key to good quality final material such as the molar ratio of metal nanoparticles to copper precursor, the molar weight of the polymer-stabilizer, the two-step order and the size of the metal particle. In fact, when smaller metal particles (5 nm) were used as in the case of Pt, the metal NPs decorated the Cu_2O nanocubes sides.

P15

A low surface impedance and high field homogeneity hybrid REBaCuO-Cu Coating for beam screens in particle accelerators

G. T. Telles[1], A. Romanov[1], N. Lamas[1], P. Krkotic[2,3], J. O'Callaghan[2], M. Pont[2], S. Calatroni[4], T. Puig[1], X. Granados[1], J. Gutierrez[1]

1 Institut de Ciència de Materials de Barcelona (ICMAB - CSIC), Campus de la UAB, Carrer dels Til·lers, s/n, 08193 Bellaterra, Barcelona, Spain

2 ALBA Synchrotron Light Source, Carrer de la Llum, 2, 26, 08290 Cerdanyola del Vallès, Barcelona, Spain

3 Universitat Politècnica De Catalunya (UPC), Carrer de Jordi Girona, 31, 08034 Barcelona, Spain

4 CERN Technology Department, Espl. des Particules 1, 1211 Meyrin, Switzerland

gtelles.es@icmab.es

CERN's future circular collider (FCC-hh) is the most ambitious scenario for a post LHC machine. It will operate as a 100 km acceleration ring where 16T magnets will steer proton bunches producing center-of-mass collision energies of 100TeV. In order to protect the superconducting magnets, the 35.4W/m/beam synchrotron radiation emitted by the protons will be absorbed by a stainless steel tube, the so called beam-screen chamber, held at a temperature window of 40-60K. Image currents will be induced into the steel walls of the beam-screen endangering the beam stability. To counteract this effect, our consortium explores the possibility to coat the interior of a beam-screen chamber with a highly conductive hybrid coating made of Cu and REBaCuO (RE = rare earth) Coated Conductors (CCs). To keep the charged particles in stable trajectories, the magnetic field quality is of extreme importance inside circular accelerators; To ensure this, CERN imposes that field error must be within a few units over 10000 for the operation of the FCC-hh. In this contribution, we analyse the magnetic field disturbance and its geometric harmonics inside the beam-screen chamber due

to the REBCO. This work will explore by means of finite elements numerical analysis a broad range of possible coating geometries that comply with the field quality criterion. In particular, we focus on the moment of the proton injection which corresponds to the most demanding of the operational scenarios. We have prepared samples of the hybrid REBaCuO / Cu coating based on geometries predicted by our model that show lower than Cu surface resistance at close conditions to those found in the FCC-hh. The experiments confirm that this method can successfully generate a coating that complies with the requirements of the FCC-hh, with high field quality and low surface resistance, and that the numerical analysis can be used as a prediction tool for future proposed geometries.

P16

A-GeSe for Selector Materials: Model Preparation From First-Principles

Linda-Sheila Medondjio[1], He Xu[1,2], Miguel Pruneda[1], Alberto Garcia[3], Pablo Ordejo[1]

1 Catalan Institute of Nanoscience and Nanotechnology (ICN2-CSIC)

2 Institute of Condensed Matter and Nanosciences, Université catholique de Louvain, Louvain-la-Neuve, Belgium

3 Institute of Materials Science of Barcelona (ICMAB-CSIC), Barcelona, Spain

lmedondjio@icn2.net

The amorphous GeSe (a-GeSe) is a good candidate for the ovonic threshold switches device. Understanding of electronic property and the related structural feature is crucial for the designing and optimization of this material. The prerequisite to study the properties of amorphous materials is the identification of reliable atomic structures. To that end, we have developed realistic Density Functional Theory-based structural models of a-GeSe without resorting experimental information or adjusted interatomic potential. A series of GexSe1-x with an extended list of stoichiometry x=0.4, 0.5, 0.6 and dopants (Si, S, As, P, Te) with various concentrations (1%, 3%, 5%,7%, 10%, 15%) has been generated with the melting-and-quenching method. The structural features, including the radial distribution function, the angle distribution function, and the coordination number distributions have been calculated. The results show that there are Ge and Se clustering in Ge and Se-rich structures, respectively; the Ge-rich structures tend to have larger coordination number, opposite to the Se-rich structures. The electronic property features, including the Crystal Orbital Hamilton Populations (COHP), inverse partition ratio (IPR), the Density of States (DOS) and the local DOS have been analysed, and we try to identify the structural origin of these features. The mobility gap decreases with x, while in the x=0.6 samples, large numbers of in-gap localized states tend to form. The dopants behave similarly with their iso-valent hosting ions with some delicate differences, of which the structural and electronic origin has been also explored. These results will provide guidelines on the improvement of the memory switching performance of a-GeSe.

P17

5G/6G Microwave Devices Based on Functional Materials

Eloi Guerrero[1], Lluís Acosta[1], Carlos Caballero[1], Jordi Verdú[1] and Pedro de Paco[1]

1 Departament de Telecomunicacions i Enginyeria de Sistemes
Universitat Autònoma de Barcelona
Escola d'Enginyeria, Carrer de les Sitges S/N, 08193.

eloi.guerrero@uab.cat

Abstract 5G and 6G wireless communications call for complex and highly integrated RF front-ends working at millimeter wave frequencies. Thus, designing devices such as filters, resonators or circulators fulfilling these requirements is an extremely challenging task that requires a deep understating of both the material and the device response side. This work is located at the bridging gap between the world of functional materials and the field of microwave component design and aims to explain how microwave design knowledge can extract the maximum capabilities of a given material. As an example, thanks to microwave filter theory, accurate design techniques have been derived to design microwave acoustic filters based on different materials such as aluminum nitride or lithium niobate thin films. Also, similar knowledge can be applied to the design of microwave circulators based on novel ferrimagnetic materials. Microwave engineering can provide a link to transform novel materials into useful devices for next generation communications.

P18

Quality Assurance of the Silicon Strip Sensors for the ATLAS Inner Tracker of the LHC at CERN

Èric Bach[1], Miguel Ullán[1], Celeste Fleta[1]

1 Institute of Microelectronics of Barcelona (IMB-CNM-CSIC)

eric.bach@imb-cnm.csic.es

The pre-production of the strip sensors for the ATLAS Inner Tracker (ITk) has recently finished and the production process has already started. Nearly 22000 large area sensors will be produced over a period of roughly 4 years and a Quality Assurance (QA) strategy has been prepared to be carried out in production. While Quality Control (QC) aims to identify defects and to provide acceptance testing checks for the finished main sensors, QA focuses on providing confidence that quality requirements will be fulfilled during the whole production process. Such a process has been characterized as providing the required pre-irradiation specifications and the proper radiation hardness. From now on, the onus is on the manufacturer to rigidly stick to that qualified process. Still, sample testing with specific device-

element structures and irradiation of devices must be implemented by the ITk collaboration. The main devices that will be used by the collaboration for QA purposes are miniature strip sensors (1x1 cm2), monitor diodes (8x8 mm2) and the ATLAS test chip. The ATLAS test chip contains several test structures to monitor specific technological and device-element parameters, such as conductive layers sheet resistance; critical parameters of the device oxides such as capacitance, thickness, breakdown voltage, flat-band voltage, etc.; Si/SiO_2 interfaces charges; and strip and inter-strip electrical characteristics.

P19

Exploring the implications of ligno-suberin barriers and related metabolites for resistance against bacterial wilt in tomato

Álvaro Luis Jiménez-Jiménez [1], Anurag Kashyap [1,2] , Montserrat Capellades[1,3], Weiqi Zhang[1] , Sumithra Srinivasan[4], Anna Laromaine[4], Olga Serra[5], Mercè Figueras[5], Jorge Rencoret[6], Ana Gutiérrez[6], Marc Valls[1,7], Nuria S. Coll[1,3]

1 Centre for Research in Agricultural Genomics (CRAG), CSIC-IRTA-UAB-UB, Campus UAB, Bellaterra, Spain

2 Department of Plant Pathology, Assam Agricultural University, Jorhat, Assam 785013, India

3 Consejo Superior de Investigaciones Científicas (CSIC), Barcelona, Spain

4 Institute of Material Science of Barcelona (ICMAB), CSIC, Campus UAB, Bellaterra, Spain

5 Laboratori del Suro, Biology Department, Universitat de Girona, Campus Montilivi, Girona, Spain

6 Institute of Natural Resources and Agrobiology of Seville (IRNAS), CSIC, Seville, Spain

7 Department of Genetics, Universitat de Barcelona, Barcelona, Spain

jimenezjimenezalvaroluis@gmail.com

The soil borne pathogen Ralstonia solanacearum is the causative agent of bacterial wilt, a devastating disease for major crops of agronomic interest. This bacterium enters the plants through wounding points at the roots, reaching the vasculature, where it proliferates massively in the xylem, provoking rapid wilting. We recently characterized in our lab that the highly resistant tomato variety Hawaii 7996 responds specifically to infection with the deposition of ligno-suberin barriers and soluble related metabolites that physically restrict pathogen colonization at the root vasculature. To further understand the contributions of this strategy to disease resistance, we will engineer susceptible tomato lines for controlled suberin deposition in response to infection at tomato roots, testing this strategy for resistance against R. solanacearum.

P20

Role of the metacaspase AtMC1 in stress-triggered protein aggregate formation in plants

Nerea Ruiz-Solaní[1], Ujjal J Phukan[1], Liang Li[1], Jose M Salguero-Linares[1], Crina M Popa[1,2], Sandra M Hill[3], Marc Valls[2], Simon Stael[4], Thomas Nyström[3], **Núria S Coll[1]**

1 Centre for Research in Agricultural Genomics (CSIC-IRTA-UAB-UB), Bellaterra, Spain

2 Department of Genetics, University of Barcelona, Barcelona, Spain

3 Sahlgrenska Academy, University of Gothenburg, Gothenburg, Sweden

4 VIB-UGent Center for Plant Systems Biology, Ghent, Belgium

nerea1rs@gmail.com

Metacaspases are critical regulatory factors that have been shown to participate in cell death and cell survival processes. For example, the Arabidopsis thaliana metacaspase AtMC1 acts both as a positive regulator of pathogen-triggered programmed cell death and also has a pro-survival homeostatic function. The loss of this protein results in the accumulation of insoluble protein aggregates and in the premature senescence of older plants. However, the molecular mechanisms by which AtMC1 maintains cellular homeostasis remain unknown. In the present thesis, proteomic and microscopic analysis have revealed that AtMC1 interacts with the molecular chaperone heat shock protein (HSP) 101, a protein disaggregase that facilitates the removal of cytotoxic aggregates and is essential for surviving severe heat stress. Moreover, protein levels and intracellular distribution and dynamics of HSP101 are altered in plants lacking AtMC1. Interestingly, phenotypic analysis have also revealed that atmc1 mutant plants exhibit an enhanced thermotolerance. Together, these observations suggest an important novel role of AtMC1 in cellular homeostasis after heat stress.

P21

Dramatic drop in cell resistance through induced dipoles and bipolar electrochemistry

L. Fuentes-Rodríguez [1,2], Ll. Abad[2], E. Pujades-Otero[1], P. Gómez-Romero[3], D. Tonti1, N. Casañ-Pastor[*1],

1 Institut de Ciència de Materials de Barcelona (ICMAB-CSIC)

2 Institut de Microelectrònica de Barcelona (CNM-CSIC)

3 Catalan Institute of Nanoscience and Nanotechnology, ICN2 (CSIC-BIST)

Campus UAB, 08193 Bellaterra, Barcelona, Spain

lfuentes@icmab.es

When conducting materials are immersed in an electrolyte, induced dipoles and bipolar electrochemistry processes change the electrochemical cell characteristics. Simple

polarization effects or electric percolation had not been sufficient to explain those changes in suspensions, since those changes occur well below the electronic percolation limits. This work shows that a significant lower resistance of the cell and charge transfer effects are present even for a discrete number of non-mobile conducting pieces inserted unconnected in the blank electrolyte. Using macroscopic conducting immersed pieces, a physical mediation due to transport through the induced dipoles is observed and if redox species exist, is enhanced. The combination is considered a physicochemical mediation. Shape or geometry, as well as size of the conducting pieces and occupation of the main field lines are significant. It is relevant that the effects observed are parallel to the previously reported for carbon suspensions and slurries, and that no electronic percolation, or induced particle ordering are needed to reach those large effects.

P22

Silicon Nanowire Single Hole Transistor with Boron Quantum Dot Fabricated by Electron Beam and Focused Ion Beam Lithography Technologies

A. Kapas[1,2], D. Bricio-Blázquez[1], M. Duch[1], A. García[1], A. Guerrero[1], J. Bausells.[1],X. Borrisé[3], F. Perez-Murano[1], J. Llobet[1]

1. Institute of Microelectronics of Barcelona (IMB-CNM CSIC), Bellaterra, Catalonia, E-08193, Spain

2. Universitat Autónoma de Barcelona (UAB), Bellaterra, Catalonia, E-08193, Spain

3. Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and The BIST, Bellaterra, 08193, Catalonia, Spain

andreeaioana.kapas@e-campus.uab.cat

Abstract Single-hole transistors have been identified as a promising semiconductor approach for quantum computation devices. The fabrication of miniaturised silicon nanoelectronics sub 10 nm gate based is still challenging, opening the possibility to build quantum devices. We carefully designed a single-hole transistor made by p-type silicon nanowire, which incorporates doped silicon nanocrystal quantum dots that behaves as Coulomb Islands. The transistor fabrication method uses rapid, high resolution, scalable and reproducible processes, based on electron beam and focused gallium ion beam lithography techniques, anisotropic wet etching, and thermal processes. In previous works, we demonstrated the single-hole effect characteristics in the I/V curves at low temperature in similar devices.

P23

Synchrotron-based Fourier-transform infrared micro-spectroscopy (SR-FTIRM) fingerprint of the small anionic molecule Cobaltabisdicarbollide uptake in glioma stem cells

Miquel Nuez-Martínez[1]; Leire Pedrosa[2]; Immaculada Martínez-Rovira[3]; Ibraheem Yousef[43]; Àngels Sierra[2]; Clara Viñas[1]

[1] Institut de Ciencia de Materials de` Barcelona, Consejo Superior de Investigaciones Cientıfícas, Campus Universitat Autonoma de Barcelona, 08193 Bellaterra, ` Spain

[2] Centre de Recerca Biomèdica CELLEX- CRBCPlanta 1A, Institut d'Investigacions Biomèdiques August Pi i Sunyer-IDIBAPS, Casanova,143, 08036 Barcelona,Spain

[3] MIRAS Beamline, ALBA Synchrotron Light Source, Carrer de la Llum 2-26, 08290 Cerdanyola del Vallès, Spain

mnuez@icmab.es

The anionic cobaltabis(dicarbollide) [3,3'-Co(1,2-$C_2B_9H_{11}$)2]-, [o-COSAN]-, in which Co^{3+} ion is sandwiched between two [$C_2B_9H_{11}$]2- ligands, is the most studied icosahedral metallacarborane. It possesses many possibilities to produce hydrogen and dihydrogen bonds (Cc-H···O and Cc-H···H-B or N-H···H-B, respectively), which have been proven to participate in their self-assembling, water solubility, micelle and vesicle formation.1 Boranes are essentially nontoxic due to their inertness to biochemical reactions; and the protonated and sodium salt of [COSAN]- possesses the ability to readily cross biological membranes not being immediately cytotoxic, but cytostatic over the long term, and cells recover following its removal.2 These abilities make the sodium salt of cobaltabis(dicarbollide), [$Na_{\cdot 2}.5H_2O$][3,3'-Co(1,2-$C_2B_9H_{11}$)2], Na[o-COSAN] suitable for the anti-cancer treatment Boron Neutron Capture Therapy (BNCT). In this work we studied the uptake of Na[o-COSAN] in two different phenotypes of glioma initiating cells (GICs), mesenchymal (GIC7) and proneural (PG88) GICs, using Synchrotron Radiation-FTIR microscopy facilities in MIRAS Beamline at ALBA synchrotron to analyze where the agent is located into the cell, taking advantage that cobaltabis(dicarbollide) displays a strong and characteristic B-H frequency in the Infrared range 2.600-2.500 cm-1 in which no other frequencies of organic compounds appear. Cell mapping was acquired, and Spectroscopic data were obtained from bands in the regions that corresponded to the DNA, proteins, and lipids to determine uptake of Na[o-COSAN]. These data suggest Na[o-COSAN] is sandwiched between DNA strings, 3 and is compatible with modifications in protein structure and lipid saturation. In conclusion, we show evidences that this new compound can penetrate and alter the physiology of the cells at low doses and can be reverted when the product is removed. Cycle cell analysis, cell viability and EC50 tests were performed to ensure the recovery of cells. Such results make Na[o-COSAN] suitable for BNCT treatment for GICs.

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