

AT ICMAB CAMPUS UAB BARCELONA 17-20 SEPTEMBER 2018 congresses.icmab.es/matener2018 matener@icmab.es





# WELCOME TO MATENER 2018!

The Severo Ochoa summer school "Materials for Energy" is addressed to last year undergraduate, master and PhD students, who are interested in the development of materials with energy applications. The aim of the summer school is to present the design, development and application of new materials for a wide range of energy applications.

The school includes lectures from international and local scientists, hands on and management activities. As a consequence, this Scientific School is an optimal opportunity to discover, learn and practice on material science focusing on fundamental science and applied research in the field of energy. The school is included in the Severo Ochoa activities of the center.

#### THE TOPICS ADDRESSED ARE:

• Functional and advanced nanomaterials for a clean and sustainable energy production, conversion, storage and transport

Materials for energy conversion
Photovoltaics
Thermoelectric materials
Materials for energy storage
Next generation batteries
Supercapacitors
Materials for energy transport
Superconducting materials

- · Life Cycle Analysis of materials for energy
- Advanced characterization techniques of energy materials

#### The school includes:

- » Lectures from international and local scientists
- » Hands-on activities and lab tours
- » Social activities: Science Dating
- » Flash presentations and Poster session
- » Awards for the best Flash presentations and Posters
- » COFFEE breaks and lunches

#### **MATENER2018** is online!

Use the hashtag #matener2018 for photos in Instagram, Twitter and Facebook!

# THE INSTITUTE OF MATERIALS SCIENCE OF BARCELONA

he Institute of Materials Science of Barcelona (ICMAB-CSIC) (www.icmab.es) is an internationally renowned public research institute in Advanced Functional Materials integrated in the National Research Council of Spain (CSIC). The mission of ICMAB is to generate new knowledge in Materials Science through excellent scientific research, useful for society and industry.

has 59 **ICMAB** permanent scientists, over 60 postdoctoral and over 110 PhD researchers in 8 Research Groups. The center has outstanding international competitiveness, with a large number of high impact articles and citations and European research projects participation (9 ERC grants at present). The center was awarded with the certificate of Center of Excellence "Severo Ochoa" by the Spanish Ministry in 2016.

The Strategic Research Program includes 5 mission-oriented Research Lines to face three social grand-challenges: clean and secure energy, smart and sustainable electronics and smart nanomedicine. The strategic Research Lines are: RL1: Sustainable energy conversion and storage systems; RL2: Superconductors for power applications; RL3: Oxide electronics; RL4: Molecular electronics; RL5: Multifunctional nanostructured biomaterials.

One of the main ICMAB's strategic objectives and missions is to recruit top worldwide class scientists in our fields of research with an outstanding track record. ICMAB provides facilities, state-of-the-art equipment and most importantly, excellent scientists and professionals, to assure you a rewarding career. A competitive and multidisciplinary training program is offered

to the new researchers to foster the development of a professional career, tailored to your needs.

The diversity of our students and the interdisciplinary research fields related to Materials Science ensure an enriching and inspiring working environment. If you are an enthusiastic and highly motivated researcher and would like to work in a multidisciplinary and multicultural environment, join us! We welcome applications from national and international candidates from many different disciplines and at all career levels. Feel free to contact us at info@icmab.es.

## "MATERIALS FOR ENERGY"

## RESEARCH LINES AT ICMAB

aterials science is a key player in the necessary move towards a new energy paradigm. Novel improved materials and processes will underpin a more sustainable energy generation, transport and storage. The ICMAB aims at being at the heart of this transformation producing step changing energy materials from non-toxic and Earth abundant substances and eye opening design rules both guided by deep theoretical insights and beyond state-of-theart experimental tools, and by developing high quality materials with low cost and sustainable methods.

The strategy of the "RL1: Sustainable energy conversion and storage systems", consists on focusing on emerging technologies based on disruptive materials with tangible strong potential for high performance and maximum sus-

tainability. In this way, and counting with the decades-long experience of our staff, we can make breakthrough contributions to various technologies. We strategically develop three applications to higher technology readiness levels: phothermoelectrics tovoltaics, batteries. Importantly, to enhance the fundamental understanding of energy materials that ultimately improves the concomitant device performance, a large stream of work is done at RL1 transversely, on developing theoretical and experimental characterization tools.

"RL2: Superconductors for power applications" is focused on the development of high quality superconductors at low cost through chemical methods. The RL has created a new colloidal solution approach to nanostructured high current superconductors and achieved a high degree of nanostructural and physical characterization. In addi-

tion, novel materials for low energy consumption electronic applications are being investigated with great success based on the control of the oxygen content in cuprate superconductors.

On the last day of the school (20 Sept., 3-4 pm) we will present you some of the research carried out at ICMAB in the fields of energy conversion, energy storage and energy transport.



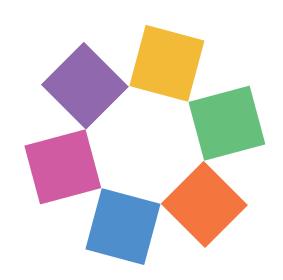








# ORGANIZERS &SUPPORT



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Alejandro Goñi

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Seminars and Training Committee





## PROGRAMME

### MONDAY 17 SEPTEMBER

08:30 - 09:30 REGISTRATION

#### **WELCOME & INTRODUCTION**

CHAIR: Rosa Palacín

09:30 - 10:00	Welcome, Xavier Obradors (ICMAB)
10:00 - 11:00	Energy in transition. A case for matter, materials and materialism, Pedro Gómez
	(ICN2, Barcelona)
11.00 - 11.30	COFFEE BREAK

#### MATERIALS FOR ENERGY CONVERSION

CHAIR: Mariano Campoy-Quiles

11:30 - 13:00	Fundamentals of photovoltaic energy conversion and conventional solar cells, Antonio Marti (IES-UPM, Madrid)
13:00 - 14:30	LUNCH
14:30 – 16:00	Non Conventional Solar Cells: Need of New Techniques for New Devices, Emilio Palomares (ICIQ, Tarragona)
16:00 - 16:30	COFFEE BREAK
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16:30 - 18:30	Hands-on experiments & Lab tours l

### TUESDAY 18 SEPTEMBER

#### **MATERIALS FOR ENERGY STORAGE**

CHAIR: Dino Tonti

09:00 – 10:30	Electrochemistry: a tutorial, John Owen (University of Southampton)		
10:30 - 11:00	COFFEE BREAK		
11:00 - 12:00	From materials to vehicle – what, why, and how?, Helena Berg (AB Libergreen,		
Goteborg)			
12:00 - 13:00	New battery technologies demand new electrolytes concepts?!, Patrik Johansson (Chalmers		
TU, Goteborg)			
13:00 - 14:30	LUNCH		
CHAIR: Nieves Casañ			
14:30 - 16:00	Supercapacitors: materials and application , Andrea Balducci (Friedrich-Schiller Uni, Jena)		
16:00 - 16:30	COFFEE BREAK		
16:30 - 18:00	Science Dating, Anna May and Ana M. López-Periago		

### WEDNESDAY 19 SEPTEMBER

#### **MATERIALS FOR ENERGY TRANSPORT**

CHAIR: Anna Palau

09:00 - 10:30 10:30 - 11:00 11:00 - 12:30	Superconductivity: A tutorial, Marina Putti (University of Genova) COFFEE BREAK Superconductivity: from materials to devices, Pascal Tixador (Institut NEEL, Grenoble	
12:30 – 13:30 13:30 – 15:00	Flash presentations (2 min) LUNCH	
15:00 – 17:00 17:00 – 19:00	Hands-on experiments & Lab tours II Poster Session + Refreshments	

### THURSDAY 20 SEPTEMBER

#### **MATERIALS FOR ENERGY CONVERSION**

CHAIR: Alejandro Goñi

09:00 – 10:30	Inorganic thermoelectric materials, Javier Rodríguez-Viejo (UAB, Barcelona)
10:30 - 11:00	COFFEE BREAK
11:00 – 12:30	Fundamentals of organic thermoelectric materials, Martijn Kemerink (IFM, Linköping)

#### **LIFE-CYCLE ANALYSIS**

CHAIR: Alejandro Goñi

12:30 - 13:30	Life Cycle Assessment applied to energy materials, Lucía Serrano (Uni Rey Juan Carlos, Madrid)
13:30 - 15:00	LUNCH

#### **WRAPPING UP AND AWARDS**

Closing, Alejandro Goñi (ICMAB)

CHAIR: Josep Fontcuberta

16:30 - 16:45

15:00 – 16:00	Materials for energy conversion: research at ICMAB, Isabel Alonso, (ICMAB) Towards post-Lithium ion batteries: improving sustainability/energy density, Roberta Verrelli (ICMAB) High temperature superconducting materials and devices at ICMAB, Teresa Puig (ICMAB)
16:00 - 16:30	Awards (Best Poster Prizes, Best Flash Prizes)

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### PEDRO GÓMEZ-ROMERO

NEO-Energy Group Leader, Catalan Institute of nanoscience and Nanotechnology, ICN2(CSIC-BIST). Campus UAB 08193 Bellaterra (Barcelona)

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# Energy in transition. A case for matter, materials and materialism

It used to be impossible, then it was judged impractical and finally it is happening. A new (and sustainable!) model of energy "generation", storage, management and consumption is in the making. A technological re-evolution which is based on true scientific revolutions made possible by people like material scientists or nanotechnologists which jobs were unheard of forty or fifty years ago.

This lecture will present an overview of the many corners of materials science involved

in the ongoing construction of novel and sustainable energy technologies and how the materials and devices emerging will need to respond to the ever-increasing demands from society. But it will also provide some analysis of this energy transition as a case study for the intertwined forces among science technology and society.

Prof. Pedro Gómez-Romero (Lic. Química (1981), Master (1982), U. de Valencia. Ph.D. in Chemistry, Georgetown University, USA, 1987, with Distinction). Investigador CSIC desde 1990 (ICMAB+ICN2). Estancia Sabática en el National Renewable Energy Laboratory, USA (1998-99). Profesor de Investigación y divulgador científico del CSIC. Group Leader del Laboratorio NEO-Energy en el ICN2 (CSIC-BIST) (2007-). Dirige proyectos sobre materiales para almacenamiento y conversión de energía, (supercondensadores, baterías de litio, celdas de flujo, energía solar térmica, nanofluidos, grafeno, materiales híbridos). Autor de diez elevado a dos (200+) publicaciones. Editor de los libros "Functional Hybrid Materials" (Wiley-VCH 2004) y "Metal

Oxides in Supercapacitors" (Elsevier, 2017). Autor de numerosas actividades de divulgación, entre ellas 4 libros (Metaevolución. La Tierra en el espejo (Celeste, 2001) (Premio Casa de las Ciencias de la Coruña, 2000), Un Planeta en busca de energía (Síntesis, 2007) Premio Internacional de Ensayo Esteban de Terreros, 2006) "Creadors de futur" (Bromera, 2016) y "Nanomundo (Materia/El País, 2016). Editor de la Web www.cienciateca.com. Fellow de la Royal Society of Chemistry (UK) (2014-). Socio fundador de la spin-off EarthDAS (1 Jun 2016-). Premio CIDETEC de investigación en Electroquímica 2017.



### ANTONIO MARTÍ

Instituto de Energía Solar – Universidad Politécnica de Madrid, ETSI Telecomunicación, Ciudad Universitaria sn, 28040 Madrid-Spain

# Fundamentals of photovoltaic energy conversion and conventional solar cells

In this lecture we review the fundamentals of energy conversion. In this respect, we will make emphasis in dismitifying the role of the electric field as the driving force for the photovoltaic effect: it is time students learn the true physics (and chemistry) behind the photovoltaic effect! By doing so we

expect to contribute to a new generation of PV researchers and funding agencies that properly focus their research and spend money. In the second part of the seminar, we will review the highlights of the main conventional solar cells such as silicon and III-Vs.

Antonio Martí graduated in Physics in 1987 by the Universidad Complutense de Madrid and doctorated in 1992 by the Universidad Politécnica de Madrid (UPM). He joined the Instituto de Energía Solar (IES) of the UPM in 1986. Together with Prof. Luque, he proposed in 1997 the intermediate band solar cell (IBSC) concept and its practical implementation with quantum dots among other options. Within IES, he has directed

the creation of IBLAB, a laboratory specialized in the characterization of intermediate band solar cells that was the first Laboratory in providing experimental proof of the operation of the IBSC concept accordingly to its postulates. In addition to IBSCs, his current research involves energy storage and other novel solar cells such aas the three terminal heterojunction bipolar solar cells.



#### FMI IO J. PALOMARES

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# Non conventional solar cells: need of new techniques for new devices

During my lecture I will present our latest results on the characterization of different type of solar cells from DSSC and OPV to MAPI using advanced photo-induced time resolved techniques1-4. Using PICE (Photo-induced charge extraction), PIT-PV (Photo-induced Transient PhotoVoltage) and other techniques, we have been able to distinguish between capacitive electronic charge, and a larger amount of charge due to the intrinsic properties of the perovskite material. Moreover, the results allow us

to compare different materials, used as hole transport materials (HTM), and the relationship between their HOMO and LUMO energy levels, the solar cell efficiency and the charge losses due to interfacial charge recombination processes occurring at the device under illumination. These techniques and the measurements carried out are key to understand the device function and improve further the efficiency and stability on perovskite MAPI based solar cells.

Emilio Palomares is ICREA Research Professor at the Institute of Chemical Research of Catalonia (ICIQ). He joined ICIQ in 2006 as a tenure-track and was appointed ICREA Researcher in 2008. In 2009 he was selected as ERC-Stg by the European Research Council. Emilio's research interests span a range of targets with emphasis on materials

for energy production and bio-applications, in the context of electron transfer processes, photovoltaic applications and nanoscience. He has received several awards including the Young Chemist Research Award by The Spanish Royal Society of Chemistry in 2006.



University of Southampton, UK j.r.owen@soton.ac.uk

#### Electrochemistry: a tutorial

This tutorial will describe the operation of a lithium ion cell and illustrate the use of basic principles of physical electrochemistry such as Faraday's, Fick's, Ohm's laws and Nernst, Butler-Volmer, Sand equations to estimate the energy and power of lithium ion cells and supercapacitors from material and interfacial properties. Standard electrochemical characterisation techniques such as cyclic voltammetry will be reviewed and contrasted with techniques more

appropriate for lithium ion cells, such as galvanostatic intermittent titration (GITT) to show how cell design and even interpretation of results for battery cells are quite different from classical electroanalytical cells. Finally, worked examples will be given to show how optimum cell performance can be predicted in theory by identifying and balancing the rate limiting processes.

John Owen obtained his first degree in Chemistry from Imperial College, London, where he also studied for his Ph.D. in Organic Electro-optic Crystals under the late E.A.D. White. He then worked on Solar Energy at the Materials and Energy Research Centre in Iran until in 1979 revolution brought him back to the Wolfson Centre for Solid State Ionics in Imperial College as Wolfson Fellow working on polymer electrolytes. In 1984 he was appointed lecturer in the Department of Chemistry and Applied Chemistry at the University

of Salford before joining the School of Chemistry at Southampton in 1990 where he is Professor of Electrochemistry. He is a Fellow of the Royal Society of Chemistry, co-founder of Nanotecture PLC spin-out company, and has authored over 100 publications on electrode and polymer electrolyte materials for batteries, supercapacitors, fuel cells and electrochromic devices.



### HELENA BERG

AB Libergreen, Goteborg, Sweden helena@libergreen.com

# From materials to vehicle – what, why, and how?

Within the current efforts of phasing out fossil fuels from the transportation sector, battery electric vehicles are considered as the prime sustainable alternative. Today, the battery concept most commonly used is the Li-ion battery technology. The main attractive properties are high energy density, enabling long driving distances, low weight and volume, enabling favourable vehicle integration modules. Being a relatively new technology in vehicle applications, still not all performance benefits have been explored. There are, however, already demands for even higher energy densities (in combination with lower cost) to design electric vehicles with same driving range as conventional vehicles. Moreover, demands

for fast-charging possibilities forces research towards new and improved battery concepts.

Today, there are several Li-ion battery materials which have different advantages and drawbacks for usage in electric vehicles. The focus of the lecture will be how different battery material properties affects the performance of electric vehicles. Moreover, how the electrodes and cells can be designed for specific usage conditions. The cell selection is therefore key for the performance of an electric vehicle, which will be discussed during the lecture. The development process of batteries from the concept stage to full-scale production will also be discussed.

Dr. Helena Berg has more the 20 years of experience in the battery field from both academia and industry, and holds a doctoral degree from Uppsala University.

For about 10 years she was one of the key persons for the development of electrified buses and trucks within the Volvo Group. As the Global Corporate Battery Specialist, she was in charge of the technology plan and had the responsibility to

follow the battery research development. Several research projects as collaborations between Volvo, academia and other industrial partners were initiated.

Since 2012, she is running her own company, Libergreen, to support companies to create strategic plans to meet future battery challenges.



#### PATRIK JOHANSSON

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# New battery technologies demand new electrolytes concepts?!

With several next generation battery (NGB) technologies emerging it could be expected that their optimized electrolytes must differ and we would need several ways to rationally optimize them. The difference could be of only a minor nature, for example by simply replacing the LiPF6 salt of lithium-ion batteries (LIBs) for NaPF6 at more or less the same concentration when creating electrolytes for sodium-ion batteries (SIBs) [1], or be much more profound, for example some of the quite special electrolytes launched for Mg-batteries [2,3].

Herein a smorgasbord of NGBs will be outlined and described and then more in detail from an electrolyte point-of-view, with examples of the opportunities and demands these create, including some more conceptual in terms of R&D tools/strategies. Design, composition and characterisation are all emphasized, but also different practical key performance indicators.

For example, within Li-S battery electrolytes the transport and solvation dynamics of polysulfides is crucial to the Li-S cell operation and at the same time

the composition of the electrolyte is itself a function of the battery state-of-charge [4]. This has by us been targeted both by non-traditional electrolyte modelling approaches [5,6] as well as operando experiments [7]. For Li-air batteries the oxygen solubility in the electrolyte is one property that needs to be addressed - and the role of the Li-salt can be crucial [8]. Overall, many Li-battery concepts diverging from LiBs (Li-S, Li-air, Li-metal) open for applying other Li-salts than the prevailing LiPF6 [9]. A special example where also the solvent must be altered are high-temperature LIBs, which can rely on ionic liquid based matrices [10]. Especially challenging are electrolytes designed for NGBs based on plating and stripping at a metal interface, not only for Li and Mg metal negatives, but also for Ca and Al-batteries [11].

Patrik Johansson received his PhD in Inorganic Chemistry 1998 from Uppsala University, Sweden.

After a postdoc with Mark Ratner and Duward Shriver at the Chemistry Department at Northwestern University, Evanston, IL, USA, he returned to Sweden and Chalmers University of Technology where he was promoted to Full Professor in Physics in 2016 (Prof. in 2012). During 2014-2015 he was Visiting Professor at LRCS-CNRS, UPJV, in Amiens, France. He has continuously aimed at combining understanding of new materials at the molecular scale, often via ab initio/DFT computational methods and IR/Raman spectroscopy, with battery concept development and real battery performance. His special interest is electrolytes; liquid, gel, polymer, and ionic liquid, especially salts and additives, for Li-ion batteries and

various novel battery technologies: Na-ion, Li-S, Mg, Ca, Al, etc. He is currently active in 3 large H2020 projects: NAIADES, HELIS and CARBAT.

In 2015 he won the BASF Creator Space Energy Storage Contest for his new ideas on Al-battery technology. He has a group of ca. 12 PhD students and postdocs, takes part in several national and international projects, many involving Swedish and European industry. He is since Jan 1st 2018 co-director of CNRS FR 3104 ALISTORE-ERI; Europe's largest industry-academia network within the field of modern batteries. He has published >135 scientific papers, written 5 book-chapters, and is Vice Head of Division for Condensed Matter Physics.



#### ANDREA BALDUCCI

Friedrich-Schiller, University of Jena, Germany

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# Supercapacitors: materials and application

Supercapacitors can be charged and discharged in seconds (or less) and display high power (10 kW·kg-¹) and an outstanding cycle life (up to one million of cycles). The energy of these devices is in the order of 8-9 Wh·kg-¹. Thanks to these properties, supercapacitors are nowadays considered the devices of choice for many high-power applications.

In this lecture several aspects related to supercapacitors will be considered. Initially, the need of high power devices in our daily life and the use of supercapacitors in our society will be discussed. Afterward, the physical and chemical processes which can be utilized for the realization of high power devices will be considered, and their influence on the electrochemical behaviour of electrochemical devices will be analysed. The active and inactive materials as well as the electrolytes used in supercapacitors will be examined in detail. Finally, the future challenges on this technology will be addressed.

Andrea Balducci is Professor for "Applied Electrochemistry" at the Institute for Technical Chemistry and Environmental Chemistry and at the Center for Energy and Environmental Chemistry Jena (CEEC Jena) of the Friedrich-Schiller University Jena, Germany. Prof. Balducci

is working on the development of innovative and safer electrolytes and materials (active and inactive) for energy storage devices, especially supercapacitors and batteries. He is author/coauthor of more than 110 publications.



#### MARINA **PUTTI**

Università di Genova, Dipartimento di Fisica Via Dodecaneso, 33, Genova, Italy putti@fisica.unige.it

#### Superconductivity: a tutorial

Anyone who is interested in science has heard about the phenomenon of superconductivity, often also in science fiction books and films (an example is the very popular movie, Avatar). Superconductivity is a quantum phenomenon, which exhibits spectacular properties with important consequences on macroscopic scale. The first one consists in the cancellation of the electrical resistance which has among its most direct consequences the possibility of having current transport on long distances without dissipation; the latter is the expulsion of the magnetic field, which generates great magnetic moments, able to levitate extremely large masses like the coaches of a train. The only contraindication is that these properties appear below a certain temperature, generally very low. Even today, more than a century after its discovery in Leyden in 1912 by Kamerlingh Onnes,

superconductivity continues to attract the interest of the scientific and technological world, in order to discover new superconducting materials with increasingly high critical temperature, understand their mechanisms and develop new applications. Just the recent past has shown us that the challenge to achieve superconductivity at room temperature is still open, but also that the properties that make a material suitable for applications can conflict with the demand for high Tc.

During the lecture the history of these 100 years of superconductivity will be reviewed, the fundamental properties and the main mechanisms underlying this phenomenon will be described, a review of the most interesting superconducting materials and their properties will be presented.

Marina Putti is Associate Professor at University of Genova. Her research activity was initially devoted to the experimental study of transport and thermal properties of superconducting materials. In subsequent years, she has been actively collaborating with US Japanese and European colleagues, in the exploration of the potential of novel superconducting materials like MgB2 anf Iron-based superconductors. On this topic, she has played a leading role at national and international level. Indeed she coordinated a European Project (FP7) coordinated with Japan

and a bilateral project Italy-USA. She co-chaired the 11th European Conference on Applied Superconductivity (EUCAS), whichtook place in Lyon in September 2013.

She published more than 210 papers on International Journals, which have been cited around 4000 times. Her research activity is internationally recognized, as evidenced by the numerous invitations to conferences including plenary lectures at the main conferences on applied superconductivity.



#### PASCAL TIXADOR

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# Large Scale Applied Superconductivity

Superconductivity is a particular state whose most spectacular property is the total absence of resistivity under a given temperature called Super-con-duc-ting temperature. materials are then perfect electrical conductors but they are not ideal since they have to be cooled at low temperatures to show their extraordinary properties. Mainly used to produce magnetic flux densities, superconductors have to carry high current densities under strong magnetic fields. The first superconductors with this ability date from the end of the fifties so that applied superconductivity began in the sixties, fifty years after superconductivity discovery (1911). A market has developed itself but it remains a niche market (about 5 000 M€ worldwide). The most popular application with more than 40 000 machines throughout the world is the MRI (Magnetic Resonance Imaging) machines, fantastic tool for physicians to investigate our soft tissues. The discovery of high Tc superconductors (HTS) in 1986 foreshadowed a revolution ("The super-con-duc-tivity revolution", Times magazine, 1987), but this revolution did not yet take place. HTS have proved extremely complex due to their anisotropy inter alia and difficult to implement industrially with high performances. The challenge is nearly to produce km long crystal! A lot of researches and developments in the world have led despite the adversity to the pre industrial production of long lengths of REBCO HTS tapes by several companies with some different routes. There is still plenty of space for improvements but these tapes have reached the stage to be used in applications and the first superconducting devices appear in real environment such as fault current limiters or wind generators.

After historical references this lecture will present the superconductivity for large scale applications, superconducting materials mainly the REBCO tapes, which concentrate the main R & D worldwide. It will end with large scale applications with a focus about Fault Current

Limiter (FCL).

After a long time at CNRS (French National Center for Scientific Research), he has been appointed as a full professor at Grenoble Institute of Technology since 2007. Pascal Tixador's main research fields are superconducting large scale applications from the device design to its construction and all tests, most of the time in industrial partnership. He is co-author of 150 peer review papers and 16 patents. He works in close collaboration with researchers involved in the material elaboration.

He was the secretary of ESAS, the European Society for Applied Superconductivity and the chairman of the 12th EUropean Conference on Applied Superconductivity (EUCAS), which took place in Lyon in September 2015, and gathered more than 1000 people, 50 % outside Europe. He is the coordinator of FASTGRID H2020 project.



### JAVIER RODRÍGUEZ VIEJO

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# Inorganic thermoelectric materials

Thermoelectric materials have the capability of converting heat into electricity. However, the efficiency of this conversion is inherently low due to the lack of materials that simultaneously exhibit high electrical conductivity, σ, and Seebeck coefficient, S, and low thermal conductivity, k. The cross-coupling of these parameters inhibits the increase of the figure of merit, a parameter defined as  $Z=(S2*\sigma)/k$ , that is used to determine the goodness of a TE material. In this talk we will describe suitable approaches to overcome the correlation between electrical and thermal conductivities, achieving electron transmitting and phonon blocking structures, that is materials with both high σ and low k. I will discuss some relevant strategies of phonon engineering to

reduce the thermal conductivity by analyzing the impact on each component of the phonon thermal conductivity, i.e., specific heat, phonon group velocity, and mean free path. The numerator of the figure of merit, known as the power factor, can also be modified to improve the electrical properties by manipulating the carrier concentration and the band structure of materials. We will review some of the families of materials and nanostructures that are promising candidates to become active thermoelectric materials in real TE applications. To end we will also briefly examine some TE devices and their current applications as generators or as sensors.

Javier Rodríguez Viejo is Full Professor of Applied Physics at the Universidad Autónoma de Barcelona (UAB) and leads the Nanomaterials and Microsystems research group at UAB and the Grupo de Física i Enginyeria de Materials (a joint group between GNaM-UAB and researchers at UPC and IMB-CNM-CSIC), 2017SGR1578. He performed the experimental part of his doctoral thesis at the 'Institut des Materiaux et Procedés' CNRS, Odeillo, France and received his PhD in Physics from UAB in 1992. Prior to his present position he was a posdoctoral fellow at the Massachusetts Institute of Technology working on the synthesis of highly-luminescent CdSe(ZnS) quantum dots and the deposition of thin film quantum dot composites by electrospray organometallic chemical vapor deposition. His research in this field resulted in several patents and papers, one of those being among the most highly cited papers in semiconductor nanoparticles. He has coauthored around 110 scientific papers in ISI journals and 7 patents, three of them under exploitation. He has participated in 43 competitive public research projects being the Principal Investigator in 27 of

them. He has also leaded 6 projects with private funding. His actual research interests revolve around thermal properties of materials at the nanoscale, particularly focusing in the physics of glasses and in thermal transport and thermoelectricity in semiconductors and nanostructured materials. He currently gives lectures at an undergraduate and graduate at UAB level on Physics, Physics of Nanomaterials and Phase Transformations and is actively engaged in the PhD programs of the Physics Department (Physics, Materials Science and Nanoscience and Nanotechnology). He was the supervisor of the Department for the PhD Program during the period 2003-2008. He has already supervised 14 (3 current) PhD students. Javier Rodriguez was the Vicedirectror of MATGAS, a non-profit research organization with partnership from Air Products, UAB and CSIC, representing UAB from March 2008 to April2015. Javier is co-founder of FutureSiSens SL, a start-up devoted to the development and commercialization of new thermoelectric-based sensors.

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#### MARTIJN KEMERINK

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# Fundamentals of organic thermoelectric materials

In this lecture I aim to give an understanding of the basics of the charge and energy transport in typical organic semiconductors that could form the basis of nextgeneration thermoelectric generators (TEG). Starting from (causes for) energetic disorder, I will introduce various ways of describing conductivity and thermopower in organic semiconductors and discuss their

applicability range. In addition, I will speak about the non-trivial effects of doping on the above. I will conclude with a discussion of what can and cannot be done to optimize the performance of organic thermoelectrics and highlight some open questions. If time permits I will also speak about cost aspects of organic TEG.

I obtained a Master degree in Applied Physics from Eindhoven University of Technology in the Netherlands in 1993. In 1998 I received a PhD from the same university on (inorganic) III/V semiconductors. After that I was awarded a 5-year post-doctoral fellowship from the Netherlands Academy of Arts and Sciences (KNAW) to work on scanning tunneling spectroscopy and STM-induced luminescence. During this fellowship I shifted my attention from inorganic, highly crystalline semiconductors to organic, amorphous or polycrystalline semiconductors. I became assistant professor in 2003 and associate professor in 2009. As of 2014 I have been

appointed full professor in Applied Physics at the Department of Physics, Chemistry and Biology (IFM) at Linköping University in Sweden, where I lead the group Complex Materials and Devices (CoMaDe).

My research interests range from fundamental charge and energy transport in disordered, mostly organic semiconductors, to device concepts and applications based on these materials. Current research topics include organic solar cells, thermoelectrics and ferroelectrics as well as ratchets. Our approach is typically a combination of experiments and numerical modeling.



### LUCÍA SERRANO

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# Life Cycle Assessment applied to energy materials

The production of materials for energy generation implies impact on the human health and ecosystems. These impacts are produced due to the required resources and processes. Life Cycle Assessment studies concluded these results, which turns into positive impacts when applied to renewable energy generators. LCA is a structured method of quantifying material and energy flows and their associated emissions caused in the life cycle of goods and services. The ISO 14040 and 14044 standards provides

the LCA methodology framework. LCA have been widely applied to renewable energies, and goods and services in general, in order to reduce and identify their environmental impacts. It is used also to decrease the costs. The application of LCA to renewable energy generators shows their advantages, costs and savings, giving a wider picture of their role in our fight against climate change and the convenience of their use.

Lucía Serrano is lecturer at University King Juan Carlos in Madrid. She enjoyed a postdoc fellowship at Imperial College London, as part of Prof Natalie Stingelin research group in the Department of Materials. She completed her PhD on 2014, which focuses on the analysis of the performance and sustainability of photovoltaic systems. She holds

an MSc on Computing Science, has published several articles and contributed to national and international conferences on the subject of Life Cycle Assessment and environmental impact of renewable energies.



#### ISABEL **ALONSO**

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# Materials for energy conversion: research at ICMAB

In this talk I will review activities of researchers at ICMAB focused on the two topics of the school related to energy conversion.

There is a very important activity in materials for photovoltaic (PV) technologies as renewable sources to achieve a clean, reliable, and affordable electricity system for the future. Different emerging PV materials for third generation solar cells are investigated including organic, hybrid halide perovskites and ferroelectric oxide perovskites. In addition, advanced photonic architectures for boosting light harvesting are also studied and applied to improve the intrinsic performance of the designed devices.

Research in thermoelectric materials is also a strong focus at ICMAB. Thermoelectric generators can be used as power elements of small devices in the internet of things as well as for wearable applications. Moreover, they could also increase energy efficiency by recycling wasted heat in most human activities or directly from the sun. Different materials are investigated to target two temperature ranges: At high temperatures nanostructured silicon/germanium systems are considered, whereas for low temperature applications organic and hybrid based thermoelectrics come into play. Potential synergetic effects in hybrid organic-inorganic systems are also being investigated. Related to this topic, the important subject of nanoscale thermal transport is addressed by developing new experimental and theoretical tools.

M. I. Alonso obtained her BS and MS degrees in Physics from the Autonomous University of Barcelona in 1984 and 1985, respectively. Subsequently she conducted research at the Max-Planck-Institute for Solid State Research in Stuttgart (Germany) and received her Dr. rer. Nat. (Ph. D.) in Natural Sciences (specialty Solid State Physics) in 1989 from the University of Stuttgart. Between 1990 and 1995 she was a postdoc at the CSIC Microelectronics Institute of Madrid, at the Materials Science Institute of Barcelona (ICMAB), and at the Paul-Drude Institute of Berlin. Since 1996 she has been staff research scientist at the ICMAB, where she is in charge of the SiGe-

molecular beam epitaxy (MBE) facility and is Head of the Nanostructured Materials Department since 2006. She is a materials physicist interested in semiconducting structures (inorganic, organic, and hybrid) that can contribute to expand the development of modern optoelectronic, energy-related, and sensing devices. Her core expertise is the MBE growth of SiGe structures and the use of optical spectroscopy, mainly ellipsometry, Raman scattering, and photoluminescence to gain deep insights into the structure-property nexus of materials.



#### ROBERTA VERRELLI

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# Towards post-Lithium ion batteries: improving sustainability/energy density

The ever-growing demand for high energy density portable electronics and the large-scale diffusion of electric vehicles and grid storage in parallel with renewable energy sources challenge the worldwide battery market to achieve maximum performances at the lowest cost and environmental impact. While the cost of the Li-ion battery (LIB) technology has been reduced, Li-ion batteries are slowly reaching fundamental limits in terms of performance. Furthermore, debates on the risk of limited lithium supply prompt to the development of more sustainable battery chemistries.

One of the most appealing choices is represented by the Na-ion technology which may in principle yield figures of merit comparable to those of Li-ion at a lower cost and thus be suitable for larger scale applications.[1] Moreover, faster progress is expected as the know-how acquired for Li-ion can be easily imported in view of the chemical similarity of both concepts.

An alternative way to bring about breakthroughs in terms of energy density would be to use lithium metal as anode (3800 mAh/g capacity instead of 372 mAh/g for graphite typically used for Li-ion). Coupling this with air cathodes would enable to reach 5 times the energy

density with the Li-ion technology. Nonetheless, the practical development of this technology is complex as stable electrolytes are needed and understanding and controlling the oxygen redox reactions at the porous cathode is a major task.[2]

Another attractive choice is to combine both the approaches and to develop batteries based on naturally abundant, multivalent metal anodes in replacement of Li. The use of light metals such as Ca [3] and Mg couples the advantages of high theoretical volumetric capacity with natural abundance, low cost, ease of handling and safety. Furthermore, the use of divalent charge carriers accounts for a two-fold increase in achievable energy density with respect to Li+ for equal amounts of reacted ions.

An overview of the fundamental research carried out at ICMAB towards the development of a post lithiumion battery technology is presented, with a critical focus on the prospects and bottlenecks related to the achievement of batteries with improved energy density and sustainability.

Roberta Verrelli graduated in Chemistry in 2012 at "Sapienza" University of Rome. She obtained her PhD in Chemical Sciences in 2015 from the same University, with a thesis on the development of alternative configurations for lithium-ion batteries, under the supervision of Prof. B. Scrosati and Prof. J. Hassoun.

In 2016 she joined the Solid State Chemistry group

at ICMAB (Barcelona) as Post-Doctoral Fellow. Her research activity, carried out in the group led by Prof. M. R. Palacín, targets the development of host electrode materials for application in post lithium-ion energy storage systems and, specifically, in Mg and Ca batteries.

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#### TERESA PUIG

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# High temperature superconducting materials and devices at ICMAB

Superconducting materials are unique materials that are able to carry large currents without losses even at large magnetic fields or sense very small magnetic fields. These properties are maintained below a critical temperature that for high temperature superconducting cuprate materials is 92 K. Their integration into devices depend on the ability to fabricate high-current longlength flexibles epitaxial tapes at low cost or the ability to nanofabricate devices on films and making them compatible with microelectronics technology. this presentation I'll briefly present the research topics we are developing at ICMAB regarding superconducting materials for

energy applications. I intend to give a flavor of the global aspects that we tackle in materials preparation using chemical solution deposition and ink jet printing, relevance of advanced characterization for correlating microstructure and properties, as well as the different approximations we are working to integrate high temperature superconducting materials in devices. In particular, I will present new approaches to evaluate their potentiality in low energy consumption memory electronics devices and the integration of tapes in energy power devices as well as in future accelerators.

Prof. Teresa Puig studied Physics at UAB and got her PhD in Physics in 1994. Upon 4 years of research experience abroad, she integrated to ICMAB-CSIC. In 2000 she got a Tenured Research position and since 2010 she is Research Professor. Since 2008 she's leading the Superconducting materials and large scale nanostructures group at ICMAB. She's published 290 article, supervised 17 PhD Thesis and filed 11 patents. In 2010 she co-funded OXOLUTIA spin-off where many of research results from the group are transferred. She has been PI of many national and European projects and recently she was granted an Advanced ERC grant. She has received several awards, the

most recent is the Barcelona City 2015 award on Experimental Science and Technology. In the last 10 years she's has been at the editorial board of "Superconducting Science and Technology" IOP journal and at the executive board of the European Society of Applied Superconductivity. She entered in research during her physics degree when High Temperature Superconductors where discovered and since then she has been working to understand them and making them better to integrated them into our society. Her scientific interests also extends to other functional properties of complex oxides.



# HANDS-ON ACTIVITIES AND LAB TOURS

ands-on activities will be on Monday, 17 September, from 4:30 to 6.30 pm, and on Wednesday, 19 September, from 3 to 5 pm.

Hands-on activities will consist of 2 hours of laboratory experiments in groups of 6-7 students. You will be able to choose among the following activities:

#### Fabrication and testing of a Li-intercalation battery (Rafael Trocoli and Dino Tonti)

The students will assemble and evaluate a hybrid battery based on Liintercalation cathode, spinel LiMn2O4, and Zn anode in a mixed aqueous electrolyte, starting from the electrodes preparation and finishing with electrochemical analysis. They will be trained in all the steps through the preparation of the battery, discussing the advantages and disadvantages of the different methods to prepare electrodes, the selection of the additives, type of current collector, and techniques for electrochemical evaluation. Different cells geometries will be employed as well as the electrochemical response of the batteries built by every student will be evaluated.

### Superconducting levitation (Alejandro Fernández and Anna Palau)

This activity will provide a vivid visualization of superconducting levitation. Several experiments will be conducted by placing a magnet on top of a superconductor (which will be cooled in liquid nitrogen). As predicted by the Meissner Effect, the magnet will levitate when the temperature of the superconductor falls below its Critical Temperature. In particular, the experiment will illustrate the case of a frictionless magnetic bearing and a superconducting train levitating above a magnetic track, reducing friction with the wheels, allowing the train to travel faster with less energy.

#### Electrochemistry of metal-air batteries (Nieves Casañ and Dino Tonti)

Zn/O2 batteries in aqueous media are the easiest way of visualizing what electrochemical energy storage offers. The use of a reducing material (Zn) and an oxidizing element (O2) renders one of the most promising, even if old, systems. The experiment will involve setting a cell, and evaluating electrochemical parameters (voltage, current...)

### Materials characterization by optical spectroscopy (Alejandro Goñi)

The power of Raman scattering and photoluminescence (PL) spectroscopy as characterization tools of different material properties such as chemical composition, strain status, band gap related properties, etc. will be demonstrated using different organic as well as inorganic semiconductors as examples.

## Turn heat into electricity: TE Demonstration (Bernhard Dörling and José P. Jurado)

This hands-on activity will consist of two parts: TE materials characterization and a hands-on demonstration of commerical TE Generators in action. In the first part, we will demonstrate the thermoelectric effect using a fan, a Peltier unit, and cold and hot water. Then, we will explain what makes a good thermoelectric material showing how to measure thermal conductivity, Seebeck coefficient and electrical conductivity.

### Organic photovoltaics (Aurelien Viterisi)

The PV workshop will consist in fabricating and characterising organic photovoltaic devices. Activities include cleaning of indium tin oxide (ITO) coated glass substrates, the deposition via blade coating of thin layers of zinc oxide nanoparticles, followed by the deposition of light absorbing layers. The process will be completed through the evaporation of the molybdenum oxide and Ag cathodes. The I-V characteristics of the produced devices will be finally measured.

## SCIENCE DATING

articipants will have the opportunity to interact with their colleagues in this social activity, which will take place on Tuesday, 18 September, from 4:30 to 6:30 pm.

We only ask you to come ready to talk about your research and open to new ideas. We are you will enjoy it!



# FLASH PRESENTATIONS AND POSTER SESSIONS

his summer school gives the opportunity to its participants to present their research in a poster format, and for those more adventurous in a 2-min flash presentation. There will be awards for the best ones!

#### **POSTERS**

- Giving a description of your research is the purpose of the poster
- The main goal is explaining clearly in what you are researching, how, and why
- All posters should be printed in DIN A0 in order to make its exhibition and presentation easier. Posters should be printed in portrait orientation (vertical).
- There will be 2 awards for the best posters.
- The poster session will be on Wednesday, 19 September, from 5-7 pm. We recommend you all to be there and to ask questions to your colleagues.

#### **FLASH PRESENTATIONS:**

· Your talk must be dynamic. Your

goal is to clearly explain what you do, how and why.

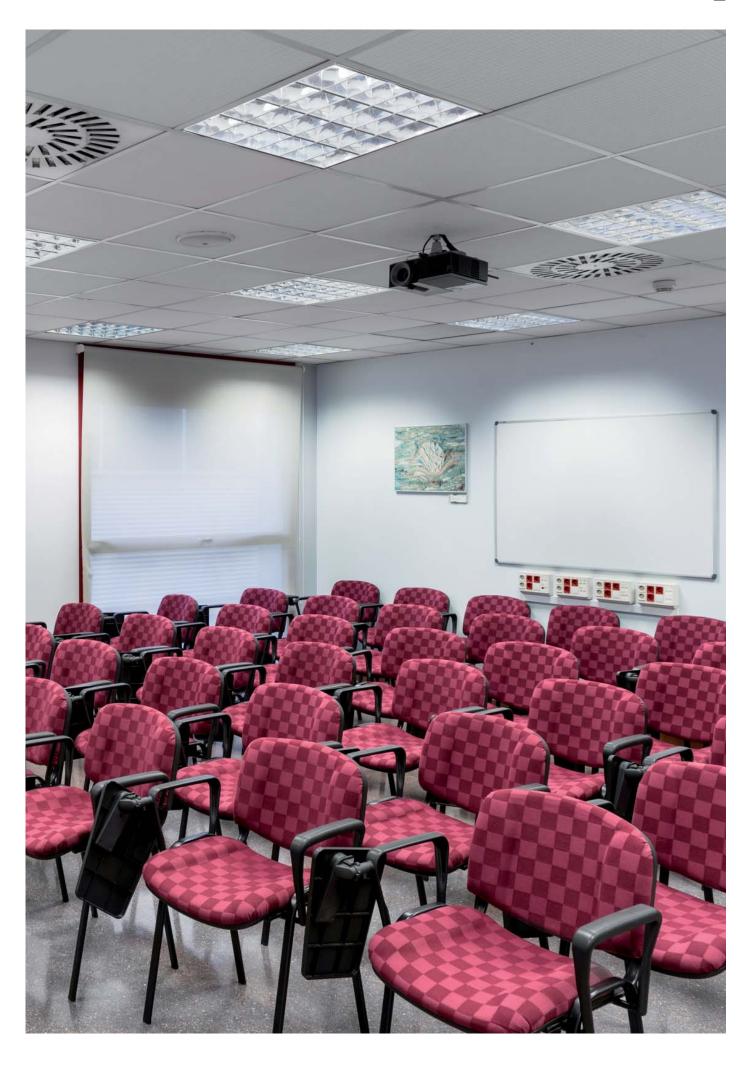
- Talks are 2 minutes long: use a minimum amount of slides (1-2) and do not fill them with a lot of text.
- Big advice: rehearse. Rehearsals will allow you to identify possible issues such as too many slides or too long/short/abstruse talk and you will feel more relaxed and ready to give the talk.
- There will be 2 awards for the best flash presentations.
- Only those already having a poster can choose to present a flash talk.
- The flash presentations will be on Wednesday, 19 September, between 12:30-1:30 pm. We encourage you all to be there.

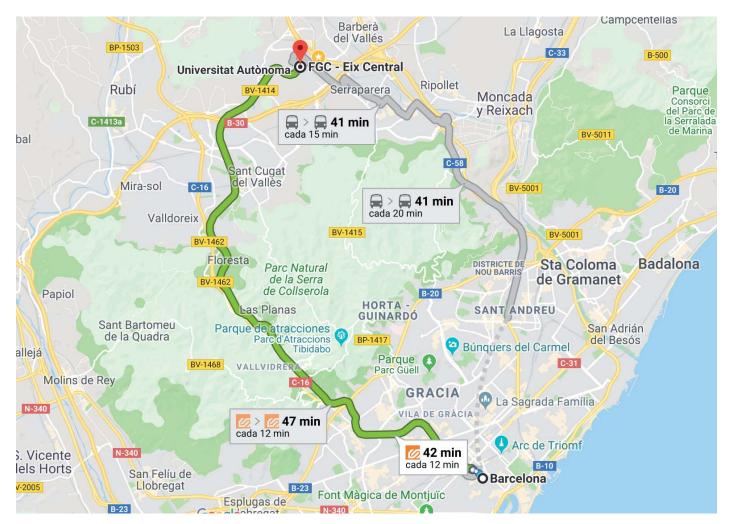
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## **VENUE**



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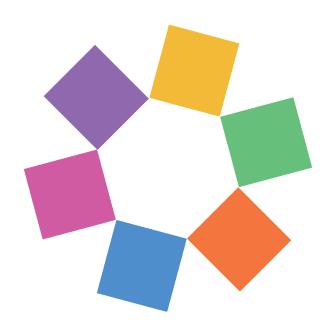
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## **NOTES**

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