ICMAB PhD PROGRAMME
SEVERO OCHOA FELLOWSHIPS

About

ICMAB-CSIC 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.

ICMAB has 62 permanent and 155 non-permanent scientists and a total of 270 people divided in eight Research Groups. The center has outstanding international competitiveness, with a large number of high impact articles and citations and European research projects participation (5 ERC grants at present), with the strongest international leadership position in the specific domains of Functional molecular, supramolecular and oxide materials. The center has been recently awarded with the label of Center of Excellence “Severo Ochoa” by the Spanish Ministry.

The Strategic Research Program includes five 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: 1/ Energy storage and conversion; 2/ Superconductors for power applications; 3/ Oxide electronics; 4/ Molecular electronics; 5/ Multifunctional nanostructured biomaterials.

The ICMAB - CSIC is one of the top research institutions named as a Severo Ochoa Research Centre by the Ministry of Economy and Competitiveness (MINECO) in charge of research and innovation policy in Spain, which recognizes excellence at the highest international level in terms of research, training, human resources, outreach and technology transfer. The Severo Ochoa award provides 4M€ over 2016-2019 to implement ICMAB’s Research and Human Resources Programmes.

Eligibility

- Candidates should be ready to enter an official doctoral programme in September 2018 (under Spanish Law). By this time, they must have obtained a university degree and a master degree; or must hold an official university qualification from a country of the European Higher Education Area with a minimum of 300 ECTS of official university studies, of which at least 60 are at masters’ level.
- Candidates must have a strong commitment to scientific research and an excellent academic record.
- Candidates must have good working knowledge of English.

How to apply:

From 18th September 2018 until 11th October 2018, an online application form will be available through the ICMAB webpage.

You will be required to provide the following information in your application:

- Personal data and CV
- Covering letter, including motivation for applying
- A copy of your Certified Academic Record, showing grades obtained (degree and masters). If these are not in Catalan, Spanish or English, applicants should attach an official translation in one of these languages

Contact:

If you have further questions, or if there are particular issues regarding your application, please contact: gestio-icmab@icmab.es

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PhD Research Topics and Projects

MATERIALS FOR ENERGY STORAGE OR CONVERSION

All-oxide photovoltaics by cost-efficient chemical routes
Mariona Coll

RESEARCH PROJECT / RESEARCH GROUP DESCRIPTION

Solar photovoltaics (PV) is a key technology for the global energy transition; solar power could provide 15% of Europe's electricity by 2030. Despite commercial Silicon PV modules have been remarkably successful they present some concerns to meet the energy demands: efficiency, life and performance with time. An all-oxide PV approach is very attractive due to the chemical, mechanical and thermal stability, nontoxicity and **abundance** of many metal oxides that allow preparation by cost-effective and **scalable** techniques. The use **of ferroelectric perovskite oxides** (FEPO) as a stable photoactive layer has opened up a **ground-breaking** new arena of **research**. They present an **alternative mechanism** for solar energy conversion that could surpass the fundamental **efficiency** limits of conventional semiconductors. Unfortunately, most FEPO are wide-band gap materials (use only 8-20% of the solar spectrum) and present poor charge transport properties.

The main goal of this project is to develop an **all-oxide device** based on FEPO with **improved light absorption** and **carrier extraction** using abundant and lead-free materials by low cost and scalable chemical methodologies. This project will build on recent results where it has been observed that cobalt substitution in ferroelectric BiFeO3 allows band gap tunability and remarkable improvement in photocurrent.

In order to unlock the full potential of the BiFe1-xCoxO3 (BFCO) system and gain new insight on its PV mechanism, improved and simplified innovative architectures based on compositional tuning of BFCO and interface engineering will be developed.

The project will be carried out at SUMAN group having wide experience on the preparation and characterization of functional complex oxide thin films and nanostructures by chemical methodologies with the aim to understand the composition-nanostructure-property relationship for energy-related applications. This project will be carried out in collaboration with Dr. M. Campoy-Quiles (NANOPTO Group). He will provide optical characterization and perform advanced photovoltaic evaluation in selected promising candidates

JOB POSITION DESCRIPTION

The student will be trained on cost-effective chemical deposition techniques (combining solution processing and atomic layer deposition) to prepare complex oxide thin films with atomic control. The student will also be trained on characterizing the structure, morphology and chemical composition of the developed films by means of xray diffraction, scanning electron microscopy, atomic force microscopy and x-ray photoelectron spectroscopy, respectively. Optical characterization and PV evaluation will be carried out in collaboration with NANOPTO group. The student will also be trained on dissemination and communication

activities. Attendance to national/international workshops and
meetings will be considered according to the work progress.
The main tasks will be:
A. Synthesize BFCO active material with graded composition in order to match the sun spectrum and achieve efficient charge extraction in a single photoactive layer.
B. Develop new metal oxide layers with superior charge transporting ability specifically designed to complement the BFCO active layer.
C. Fabricate all-oxide devices with enhanced efficiency
This work will provide a novel family of promising materials that can revolutionize the existing PV technologies and allow better understanding of the alternative PV mechanism that produce the ferroelectric materials.

Skills Requirements:

- PhD in Materials Science, Physics or Chemistry
- Background and experience in preparation of oxide thin films and structural
- characterization will be useful
- High motivation and aptitudes to work in collaborative groups
- High level in written/spoken English

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Real time imaging of heat propagation at the nanoscale in quasi-2D hybrid systems
Juan Sebastián Reparaz, Maria Isabel Alonso.

RESEARCH PROJECT / RESEARCH GROUP DESCRIPTION

Nanoscale heat transport has emerged in the last 10 years as a field of increasing interest towards efficient energy regeneration. Thermoelectricity is perhaps one of the fields that has captured largest attention from the science and technology perspectives due to its possible applications to renewable energies. However, our understanding of heat transport at the nanoscale is still in development, e.g., few is known on the wave nature of heat.

In this proposal we aim to pave the way towards efficient heat manipulation. We will study heat propagation in ultraslow motion in quasi 2-dimensional (2D) hybrid systems based on suspended silicon nanomembranes and polymer thin films. We aim to investigate the development of heat waves (second sound) as well as the influence of inorganic/organic thermal boundary resistance in the resulting thermal distribution. For this purpose we will develop a full novel approach based on optical interferometry and frequency- and time-domain thermoreflectance. The samples will be imaged through this technique with high spatial resolution (about 200 nm), high temporal resolution (about 30 ps), and high temperature resolution (about 100 µK), and through reconstruction of the data we will produce a live video of the evolution of a single heat pulse. All experiments will be carried out in a pump-and-probe configuration and as a function of temperature between 5K and 600 K. The obtained thermal videos will not only be a fully new experimental development, but will be the key to understand heat propagation in these quasi 2D systems. The samples will be fabricated by combining molecular beam epitaxy for the inorganic candidate, and combined with doctor Blade and spin casting to deposit diverse polymer candidates. We expect that the successful output of this project will have impact on establishing the wave-like thermal propagation regime, as well as establishing a new optical technique to study nanoscale heat transport.

JOB POSITION DESCRIPTION

The candidate should have a background education in physics, chemistry, or engineering, and should demonstrate commitment and scientific independence. Basic knowledge on thermal transport will be valuable but not mandatory. Interest for experimental science and setups development will be positively evaluated. A good level of English (written and spoken) is required for the successful execution of the project. The candidate will have the opportunity to spend certain amount of time in foreign universities and/or research centers, which will be decided upon periodic evaluation by the supervisors. It is expected that within the project duration the candidate will develop scientific writing skills in order to publish the obtained results in international high impact journals. Finally, team work skill with the rest of the group members will be positively evaluated.

Regarding the specific tasks to be conducted:

- Development of a pump and probe imaging technique in the time- and frequency-domains simultaneously. Development of the measurement and analysis numerical tools.

- Fabrication of the samples through molecular beam epitaxy, spin casting, and Dr. Blade. General structural and chemical characterization of the samples (SEM, Raman, Optical spectroscopy, etc)

- Measurement performing in the fabricated samples and reporting: internally to the supervisors, drafting of scientific publications, and presentations in international conferences and workshops.

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Nitride materials for photocatalysis and solid state lighting
Amparo Fuertes

RESEARCH PROJECT / RESEARCH GROUP DESCRIPTION
The project of this doctoral thesis aims at the development of metal oxynitrides as new materials for two applications in energy: 1) photocatalysis under visible light for water splitting and for the decomposition of organic molecules, and 2) red luminescence for application in white LED's. The partial substitution of the anion oxide by nitride expands and tunes the physical properties of oxides, and oxynitrides are an emerging group of solids showing high dielectric constants, colossal magnetoresistance, ferroelectricity, red luminescence and visible light photocatalytic activity. (1) Nitrogen and oxygen show similar electronic and crystal chemistry features and may substitute for each other in the same crystallographic sites. Nitrogen is less electronegative and more polarizable than oxygen and the anion is more charged, then its introduction in an oxidic compound increases the covalent character of the bonds with the cations and the crystal field splitting. This results in changes in the electronic levels inducing important effects as for example decreasing the band gap in the semiconductors, which shifts to the visible light the activity of photocatalysts. Another effect is lowering the energy of the d orbitals of the rare earths, which increases the emission wavelengths of luminescent cations. Perovskite oxynitrides will be developed to produce new visible light photocatalysts for water splitting and organic reactions. (2) Silicate oxynitrides will be investigated as hosts for Eu^{2+} and Ce^{3+} luminescent materials which show large colour tuneability, low toxicity and high thermal stability. (3,4) The research group hosting the student has a long experience in the development of new nitrided materials with a diversity of properties including superconductivity, photocatalytic water splitting, colossal magnetoresistance and luminescence.
References: (1) A.Fuertes, Mat. Horizons 2 (2015), 453. (2) A.Fuertes et al, Chem. Comm. 54 (2018), 1525. (3) A.Fuertes et al, Chem. Comm., 51(2015), 2166. (4) A.Fuertes et al, J. Mat. Chem. C. 3 (2015), 11471.
JOB POSITION DESCRIPTION
The student will be trained in non conventional synthetic methods at high temperatures with strict control of atmosphere and other parameters in order to produce the targeted oxynitrides. She/He will perform the preparation of powder samples at high temperatures in nitriding atmospheres as well as the characterization of the chemical composition, crystal structure and physical properties. The investigation of the crystal structure will be performed by using X-ray diffraction, transmission electron microscopy and electron diffraction at ICMAB, and also at international facilities like the ALBA synchrotron and neutron diffraction (Institut Laue Langevin in France or ISIS in UK). The optical properties of the oxynitrides will be studied by luminescence measurements. The photocatalytic properties will be investigated in oxidation and reduction of water as well as in the decomposition of organic molecules.
Expected academic requirements and skills required for the position:

- Degree in Chemistry or Materials Science
- Academic grades will be considered in the evaluation
- Research experience (less than 4 years) will be considered in the evaluation
- High motivation for experimental research
- Working aptitudes in a collaborative group

- High level in written/spoken English

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Controlling the composition and architecture of discharge products in metal-air batteries
Dino Tonti, Andrea Sorrentino

RESEARCH PROJECT / RESEARCH GROUP DESCRIPTION

Metal/air batteries could allow 3-5 times the specific energy of current Li-ion batteries at a lower cost, making an ideal choice for electric vehicles. However, their durability is often limited, and the mechanisms that lead to their failure are generally poorly understood.

The research line lead by Dr. Dino Tonti aims to contribute to this rationalization and improve performance by combining new materials and advanced characterization.

The present work will be directed by Dr. Dino Tonti in collaboration with Dr. Andrea Sorrentino, beamline scientist at the Synchrotron ALBA, where part of the experiments will be designed and carried out.

Dr. Dino Tonti is a chemist, staff scientist at ICMAB. He has worked on surface science and optical techniques, synthesis of colloidal nanoparticles, carbons and battery materials. As CSIC responsible within the EU project LABOHR he has gained considerable insight in Li-air batteries, and remains involved in metal-air batteries within several topics: development of novel electrode architectures, study of electrolyte additives, and characterization of electrochemical processes by analysis of discharge products and in situ monitoring.

Dr. Andrea Sorrentino is scientist at MISTRAL, ALBA's transmission soft X-ray microscopy beamline. His current research interests focus on the study of samples using different techniques: cryo transmission tomography, X-ray magnetic circular dichroism and spectromicroscopy, the latter in particular on battery materials.

JOB POSITION DESCRIPTION

All battery components have strong influence on the performance, however in metal-air batteries the interplay between the design of the positive electrode, the operating conditions and the electrolyte composition is extraordinarily complex and leads to a wide range of performances. A key factor to understand the reaction mechanism and to control rechargeability is the composition and architecture of the discharge products. Combining lab- and synchrotron-based methods, this work will study the morphology and composition of products precipitated during the cell discharge, and relate them to several factors such as the electrode texture, the presence of solid or soluble catalysts or other additives in the electrolyte able to control the stability of reaction intermediates. This information will help to minimize formation of side products, and produce precipitate architectures that promote the most efficient removal.
As electrode we use bacterial cellulose, a high purity, renewable, safe and easily processable material, consisting of cross-linked nanometric fibers. After pyrolysis cellulose provides electrodes with suitable architecture, and conductivity comparable to those from carbon

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nanotubes or graphene. It provides at the same time a well-defined model system for basic studies as a scalable material for practical applications.
The student will participate to the development of more efficient metal/air batteries using different anodes and electrolytes. In particular he/she will:
• Process bacterial cellulose as functionalized binder-free electrodes
• Investigate their electrochemical behavior in batteries.
• Investigate the electrode and cell materials before, during and after operation with emphasis on imaging and spectroscopic techniques

Required degree: MSc or equivalent in Physics, Chemistry, Nanotechnology, Chemical engineering or Materials Science.
Valuable experience: electrochemical energy storage, interfacial electrochemistry, electron microscopy, x-ray absorption.

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SUPERCONDUCTORS FOR POWER APPLICATIONS

Ultrafast growth of thick superconducting epitaxial layers from transient liquids
Teresa Puig

RESEARCH PROJECT / RESEARCH GROUP DESCRIPTION

This project is part of the ERC Advanced Grant ULTRASUPERTAPE which aims to demonstrate an unprecedented approach for fabrication of low cost / high throughput / high performance High Temperature Superconducting (HTS) tapes, or Coated Conductors, to push the emerging HTS industry to market. A superconductor is a material with zero dissipation that will boost many energy applications if The breakthrough idea is the use of Transient Liquid Assisted Growth (TLAG) from low cost Chemical Solution Deposition (CSD) of Y, Ba, Cu metalorganic precursors to reach ultrafast growth rates. The key concept of TLAG-CSD relies on the ultrafast growth of the superconducting. $YBa_2Cu_3O_{7-x}$ phase through a transient liquid (100 times faster than present methods) Several routes are presently being studied for thin films. This grant faces the challenge to reach epitaxial growth of thick (>1 µm) films. The main limitation factor is the fast elimination of the barium carbonate intermediate phase. Strong knowledge on the phase diagram and epitaxial crystal growth from liquids will be essential.

These understanding will be later adapted to nanocomposite superconducting films prepared from nanoparticle colloids and to flexible technical substrates to analyse the scalability issues which will be transferred to our spin-off company.

ULTRASUPERTAPE aims to boost Coated Conductors performances up to outstanding limits at high and ultrahigh fields, by smartly designing and engineering the local strain and electronic state properties of the layers. This PhD grant will contribute to the project with the understanding of the growth mechanisms with special attention to thick layers (>1 m) also deposited by innovative Additive Manufacturing and Digital Printing methodologies using combinatorial chemistry for fast screening of critical parameters. The structural and superconducting properties of the layers obtained will be analysed with in-situ synchrotron experiments, high resolution electron microscopy and advanced superconducting characterization techniques.

JOB POSITION DESCRIPTION

One Doctoral (PhD) student position in material science, materials engineering, chemistry or chemistry engineering in the framework of the Functional Advanced Materials program for SEVERO OCHOA excellent award.

The open position has a duration of 4 years and it is in experimental material science, in the area of growth of high temperature superconducting films and nanocomposites using an outstanding ultrafast approach:

- Growth of epitaxial superconducting thick layer from a transient liquid assisted method of chemical solution deposited layers
- Understanding of epitaxial growth mechanisms

- Study of intermediate phase reaction through advanced in-situ synchrotron XRD experiments and high resolution electron microscopy of quenched samples
- Use of combinatorial chemistry approaches by innovative digital printing methodologies for fast screening of process parameters
- Adaptation of this knowledge to the growth of nanocomposites and technical flexible substrates
- Characterization of the final superconducting and structural properties

The position will involve solution chemistry, clean-room environment, ultrafast growth experimental furnaces, advanced characterization tools. This work is part of an ERC Advanced Grant.

ICMAB offers excellent conditions for PhD students, including:
- a creative, world-class interdisciplinary research environment for fundamental and applied nanoscience state-of-the-art infrastructure for the preparation and characterization of nanostructured materials.
- a highly regarded scientific education.
- a strong international nanoscience network.
- Broad knowledge on superconductivity and superconducting materials

The candidate must possess:

- Bachelor in materials science, materials engineering, chemistry or chemistry engineering and a master in any of the above degrees.

- A high level of English.

- High motivation to experimental research.

- Working aptitudes in a collaborative group.

We invite applications from excellent candidates anywhere in the world.

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OXIDE MATERIALS FOR ELECTRONICS

Strain gradients at the nanoscale: visualizing defect chemistry and electric fields
Felip Sandiumenge

RESEARCH PROJECT / RESEARCH GROUP DESCRIPTION

In nanostructured oxides, strain, defect chemistry and electric fields, commonly come together at the nanoscale, controlling functional properties. Disentangling the interplay between them, however, remains elusive owing to the difficulty of visualizing and quantifying their effects at nanoscale defect structures.

This proposal focuses on the application of transmission electron microscopy techniques to investigate the effects of local strain on: 1) defect chemistry and 2) generation of local electric fields associated to eg Schottky barriers, flexoelectric effect or screening charges at charged defects. Such local strain fields can be associated to crystalline defects such as dislocations, domain boundaries or metal/insulator interfaces, and the direct visualization of associated effects like those mentioned above remain challenging. The microscopy work proposed here combines state of the art techniques for the visualization of electric fields with subnanometer resolution, like differential phase contrast, and spectroscopic techniques like energy dispersive x-ray and electron energy loss spectroscopies. Such experiments, which require aberration correction, will be performed in laboratories abroad with whom the research group currently holds collaborations in these areas.

The research group grows up from a collaborative initiative between members of the Oxide Nanophysics Group at ICN2 (Prof. G. Catalan, group leader) and the Advanced Characterization and Nanostructured Materials Group at ICMAB-CSIC (Dr. F. Sandiumenge), and is eventually open to other ICMAB research groups sharing a similar scientific interest. The group holds long-standing expertise in the investigation of flexoelectricity and crystalline defects such as dislocations and domain boundaries in functional oxide materials, and work in collaboration with local experts in the growth of high quality oxide epitaxial films.

JOB POSITION DESCRIPTION

In a first step, the successful candidate will collaborate in the growth and optimization of materials in thin film form, containing defect structures generating local strain gradients such as for instance dislocations and misfit dislocations, domain walls in ferroelastics or ferroelectrics. Activities at this stage may include the characterization of oxide thin films by (though not necessarily all) atomic force microscopy (including conducting mode), Kelvin probe microscopy, x-ray diffraction and high resolution transmission electron microscopy using a local field emission instrument.

In a second stage, selected materials will be investigated using aberration corrected microscopes available at the Instituto de Nanociencia de Aragón-INA (Zaragoza, Spain) or Nanogune (Donostia, Spain) for atomic resolution imaging and spectroscopy. Direct visualization of electric fields with subnanometer resolution will be carried out at the Center for Electron Microscopy and Analysis – CEMAS at the Ohio State University (USA), using differential phase contrast. For more detailed information, interested candidates are encouraged to get in touch with F. Sandiumenge.

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https://departments.icmab.es/acnm/; https://icn2.cat/en/oxide-nanophysics-group

Learning from neuromorphic vision systems using time causality of optical stimuli
Gervasi Herranz

RESEARCH PROJECT / RESEARCH GROUP DESCRIPTION
We have investigated the properties of quantum wells (QWs) at the $LaAlO_3/SrTiO_3$ interface, including 2D superconductivity, Rashba spin-orbit fields and lattice vibrational modes [1-3]. More recently we uncovered persistent photoconductance (PPC), whereby the system changes its conductance in a plastic way, retaining memory from its past history, as in the case of memristors, but using light instead of electric pulses. Our most astounding discovery (yet unpublished [4]) is that light pulses can be used to replicate spike timing-dependent plasticity (STDP). STDP was proposed to emulate time causality of electro-chemical signals in biological neurons: pre-synaptic neurons spiking after post-synaptic neurons are "anti-causal" and learning is weakened; pre-synaptic neurons spiking before post-synaptic neurons are causal, reinforcing learning. STDP enables unsupervised learning, without need of labelling training data.
Our discovery is particularly relevant, as it extends the STDP concept beyond electrical stimuli to the realm optical stimuli, opening up whole new perspectives on neuromorphic engineering and in artificial vision. More specifically, our project aims at generating neuronal spikes in our physical system –e.g., using, among other approaches, RC differentiators, where R and C are defined in the QWs–. The candidate will be trained in Python-based algorithms that will help to understand how artificial networks can be designed to learn from visual inputs, with the ultimate objective of building a first design that may learn from simple visual patterns. The student will be supervised by Dr. Gervasi Herranz, whose activity can be reached through the Researcher ID: G-2770-2014

[1] Pesquera et al., Physical Review Letters 2014.
[2] Herranz et al., Nature Communications 2015.
[3] Gazquez et al., Physical Review Letters 2017.
[4] Y. Chen et al., to be submitted soon.

JOB POSITION DESCRIPTION
As described in the Research Project, the candidate will follow his/her PhD Thesis in the field of neuromorphic computation. To achieve the scientific objectives, he/she will have access to all required laboratories, all located within ICMAB premises. In particular, he/she will access our optical laboratory, which includes high-resolution microscopy using wavelengths in the visible, with accurate control of irradiance and optical stimuli controlled to timescales down the microsecond. The laboratory has deep expertise in magnetotransport and optical

characterization of quantum wells. The candidate will be responsible to
define neuromorphic devices with length scales ranging from tens of microns to submicron scales, using optical and/or electron beam lithography. The supervisor of the project will provide all the necessary means for the successful candidate to attend schools and relevant international scientific meetings and workshops. The candidate will benefit also from training in the use of Python-based algorithms to model neural networks and from international collaborations across Europe.
Candidates should be fluent in English, with a background in solid state physics and optics. Programming and mathematical skills as well as enthusiasm for Science are more than welcome.

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Ferroelectric oxides nanoengineering for enhanced photovoltaic performance.
Ignasi Fina

RESEARCH PROJECT / RESEARCH GROUP DESCRIPTION

The science behind Photovoltaics (PV) in semiconductors has been understood for decades. In the present project it is proposed to overcome the PV efficiency limits present in PV technology based on semiconductor materials exploring a peculiar kind of materials, called ferroelectric materials, that may offer a powerful new mechanism for converting light into electricity.
Ferroelectric materials are those materials that demonstrate switchable spontaneous surface charge upon application of electric field. If surface charge is not properly screened ferroelectric materials can hold a giant electric field (overpassing those appearing in semiconductor), which can potentially lead to large efficiencies, in principle forbidden for semiconductors technology.
The drawback of ferroelectric materials is their large bandgap and low carrier mobility. The most commonly followed strategy by the scientific community to overcome these issues is to investigate on new materials that can show larger absortion and larger carrier mobilities, usually at expense of the good ferroelectric properties. Another possible route is the combination of ferroelectric materials with other materials showing larger absorption. This route presents the main disadvantage of that the place where the photocarrier is generated is not the same where the electric field is present. Recent theoretical works have shown that appropriate combination of some unit cells thick layers of appropriate materials; can combine good ferroelectric properties with high absorption. These properties would be present all across the material resulting in a new uniform band diagram.
Pulsed laser deposition (PLD) in combination with Reflection high-energy electron diffraction (RHEED) to growth the proposed materials, which will allow the growth control at the atomic scale to obtain artificially nanoengenired novel ferroelectric materials with high absorption, will be used in the present project. The selected material constituents will be based on BaTiO3 which is a ferroelectric material with large polarization at room temperature and free of any toxic element that can hinder applications.

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JOB POSITION DESCRIPTION

The proposed PhD thesis will carefully address the photoelectric response of ferroelectric under different conditions using state-of-the-art characterization devices. Therefore, the PhD student will acquire knowledge on material growth and basic characterization. The PhD student will get wide experience on photoelectronic characterization, not only required for technological perspectives like the one proposed for his/her PhD thesis, also required for still emerging technological areas such as solar cells.

The student will be integrated in research synergies with groups across Europe (UK, France, Czech Rep., and Germany) and USA (California). Moreover, he will be required to attend and participate at international conferences, and trigger by himself dissemination and outreach activities. Therefore, good communication skills are mandatory.

The PhD student will be integrated to the MULFOX group at ICMAB (http://www.icmab.es) under supervision of Ignasi Fina (https://sites.google.com/site/ifinawebsite).

GROUP LEADER:

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Challenging a Nobel's prediction. Data storage with antiferromagnetic materials.
Josep Fontcuberta

RESEARCH PROJECT / RESEARCH GROUP DESCRIPTION

Ferromagnetic magnetic materials are extensively used in technology. A characteristic feature of them is that they have a net magnetization that can be detected and modified by external means and can be mapped by external probes. Therefore, ferromagnetic materials are active-responsive and visible. In contrast, antiferromagnetic materials, although also constituted by magnetic atoms, have a net zero magnetization and thus they cannot easily be controlled and are invisible to an external inspector. Probably for these reasons, antiferromagnetic materials have been largely ignored. Indeed, in the 1970 Nobel Prize Lecture for his discoveries on Magnetism, L. Néel stated: "Antiferromagnetic materials do not seem to have any application".
Now, a new life is being received by antiferromagnets. Indeed, in spite that having zero magnetization, it has been shown that they can be used to store and retrieve magnetic information, and for these findings, antiferromagnets are receiving a renewed attention [1].
Still, writing information in them is far from simple as either large magnetic fields or complex temperature cycling are required to change their magnetic state [1,2].
On the other hand, during the last few years it has been shown that the intimate coupling between charge and spin, can be broken and pure spin currents can be generated in some materials, with the additional benefit that spin do not suffer the energy costly Joule effect.
As a result of spin currents, spins can be accumulated at sample edges and the resulting magnetization can exert a magnetic torque in neighboring magnetic layers and eventually induce the switching of its magnetization direction. Indeed, it has been recently shown that this mechanism lead to efficient switching of magnetization, and thus magnetic information writing is more energy efficient.
Here again, antiferromagnetics may find a new opportunity. Indeed, it has been shown that spin currents can be transmitted in antiferromagnets and nothing precludes that their magnetic state can be modified by a spin current and consequently information can be written on them.
We know how to write information in antiferromagnets by conventional (magnetic fields & temperature) [1,2] and we also know how to measure and exploit spin currents [3,4] and we do have the necessary expertise to grow the suitable antiferromagnetic films. Therefore, we are in an excellent position to explore spin currents in antiferromagnets with the view on new concepts of more energy efficient and robust memory devices for data storage. This is the ultimate goal of this project.
The student will be supervised by Prof. Josep Fontcuberta.

JOB POSITION DESCRIPTION

The research plan includes: a) growth and fabrication of the proposed materials by using worldwide state-or-the art growth techniques, b) structural and morphological characterization by using X-ray diffraction techniques and proximity probe microscopy and c) exhaustive electric and magnetic testing using suitable magnetometers, radio-frequency magnetic resonance

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facilities and probe stations. Use of large European facilities, such as ALBA synchrotron, will be also scheduled.
This scientifically demanding project, requires a very motivate candidate with a solid back ground degree and Master on solid state physics, material's science or nano-engineering. We are seeking for a candidate enthusiastic about the job, able to fluently communicate in English and ready to travel to international scientific forums and specialization schools, and to foreign laboratories.
We expect independent minded candidate, with a solid background on materials science and solid state physics, that can contribute much to the definition of critical aspects of the project.
The candidate will joint of the MULFOX team (http://www.icmab.es/mulfox/) with a large expertise on all aspects of the work plan, excellent records of scientific production, impact and international recognition and with access to all necessary facilities for a fast progression.
Visit: MULFOX web site at http://www.icmab.es/mulfox/

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Coupled ordering phenomena in novel frustrated and magnetoelectric oxides
José Luis García Muñoz

RESEARCH PROJECT / RESEARCH GROUP DESCRIPTION

The activities of the CMEOS group at the ICMAB center on strongly correlated materials of interest in Condensed Matter research and for Information Technologies. This PhD project is focused on the fabrication and advanced characterization of novel magnetoelectric frustrated oxides. Frustration, or the inability to satisfy all interactions, leads to new fascinating phenomena and properties (quantum magnets, spin liquids, chiral spin orders, magnetoresistance, etc.). The recent discovery of new classes of frustrated materials (type-II multiferroics, MFs) in which the charge or magnetic orders and the (ferro-)electric properties are strongly coupled is attracting very much interest for fundamental research and spintronic applications because of the possibility to manipulate magnetism by electric fields and vice-versa. Selected 3d and 4d magnetic oxides with topological or exchange frustration will be grown as single-crystals or thin films, in which the appearance of particular charge/spin/orbital orders generate ferroelectricity (FE) due to spin-charge coupled effects. Some structurally simple oxides with charge modulations or chiral spin structures are receiving tremendous attention as the richness of possible magnetoelectric mechanisms greatly exceeds our expectations. Their study requires using neutron and x-ray diffraction methods, and other synchrotron techniques. One of the goals is to obtain strong coupling between the electric and magnetic order parameters as occurs in MFs with cycloidal, conical or fan magnetic phases, allowing the magnetic control and manipulation of the FE states. The MF ground-state can be modified by the application of external fields or pressure, or in strained thin films. Our group has long-standing expertise and international recognition on advanced structural and magnetic crystallography using neutron and synchrotron techniques. We combine experimental and theoretical approaches to tackle the structure-properties relationships.

JOB POSITION DESCRIPTION

This PhD project involves the fabrication and characterization of frustrated transition metal oxides with multiferroic and magnetoelectric properties, presenting a strong coupling between charge&magnetic and the ferroic orders. Selected well-ordered solid-state oxides presenting octahedral, pyramidal or tetrahedral units, in structures favoring competing charge/spin orders, will be grown as single-crystals using modern Optical Floating Zone equipment in our lab., in powder form or as epitaxial thin films. Besides using the conventional laboratory techniques and the Rietveld method for their structural characterization, the proposed project require atomic level structural, magnetic and electronic structure information that will be obtained using synchrotron techniques and neutron diffraction experiments in Large European Facilities (including ALBA). These experiments will be performed as a function of temperature, pressure and under external magnetic or electrical fields.

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Profile

- Applicants should have (or expect to obtain) a Master degree in Materials Science, Physics, Chemistry, Nanoscience, Nanotechnology or a related field.
- Academic knowledge of condensed matter physics or solid state chemistry, and some research experience will be appreciated.
- High motivation for experimental research
- Good English communication skills, and motivation to work in international environments, travel to Large European Facilities and attend specialized international schools.

References: [1] Morin et al, Nature Communications 7, 13758 (2016). [2] Cheong et al , Nat. Mater. 6, 13 (2007). [3] Y. Tokura et al, Rep. Prog. Phys. 77, 076501 (2014). Also Phys. Rev. B 97, 235129 (2018); Phys. Rev. B 96, 024409 (2017); Phys. Rev. B 96, 104435 (2017), Phys. Rev. B 94, 014411 (2016); Phys. Rev. B 85, 224419 (2012).
More information on our research can be obtained through the CMEOS website and the Researcher ID: A-7983-2015 and ORCID: 0000-0002-4174-2794. Contact us for further details.

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Nanoelement integration in oxide films for novel electronics
Alberto Pomar, Lluis Balcells

RESEARCH PROJECT / RESEARCH GROUP DESCRIPTION

Manipulation of matter at the nanoscale has been recognized by the EU as a key area to open new horizons in diverse fields as Big data, Biomedicine and Energy. In particular, a major challenge is to find efficient approaches to integrate regular patterns of nanoscale objects (atoms, clusters, ...) into large surfaces of functional materials. The feasibility of a new route to fabricate long range ordered arrays of nanoobjects based on the use of templates obtained by self assembly has been demonstrated. These nanotemplates are achieved by fine tuning of growth kinetics during the sputtering process of transition metal oxides (TMOs) thin films. Our scientific objective is to combine the unique electronic, magnetic or optical properties inherent to quasi-zero-dimensional nanostructures with the exceptional range of applications offered by TMOs used as nanotemplates (colossal magnetoresistance, ferroelectricity,…). As light-matter interaction is enhanced by the presence of nanoscale objects through electromagnetic confinement at surfaces and interfaces, the tuning of electronic properties of the template will lead to new concepts in optoelectronics.

JOB POSITION DESCRIPTION

We are looking for highly motivated candidates with a solid background in physics. The candidate will work in a rich and multidisciplinary environment at the "Advanced Characterization and Nanostructured Materials" (ACNM) group at the Materials Science Institute of Barcelona (ICMAB). The group has a long-standing record of high quality publications in the field of functional oxide materials for novel technologies. Our research is both of basic and applied character since it is aimed not only to investigate the relation between the microstructure and properties but also its potential application for the design and fabrication of novel magnetoelectronic devices. The student will be responsible for the preparation of devices consisting of nanoparticles deposited by cluster gun on top of oxide-based nanotemplates prepared by sputtering. Candidate will be in charge of the study of electronic properties of the devices.

GROUP LEADER:
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New challenges in spin-orbit physics
Benjamin Martinez

RESEARCH PROJECT / RESEARCH GROUP DESCRIPTION

Spin-orbit coupling (SOC) is a relativistic effect linking orbital and spin angular momenta of an electron that becomes significant for atoms with high atomic number. Recently research on 5d transition metal oxides (TMOs) with pronounced SOC is flourishing due to the emergence of new topological states and potential application in spintronics. In these 5d transition metal oxides, several energies scales are competing (Hubbard's interaction, Hund's coupling, SOC, crystal field and electron kinetic energy) and a rich family of behaviors has been revealed. Moreover, SOC is at the heart of manipulating spin solely by electric fields, an attractive pathway for designing electronic devices, in particular magnetic random access memories with reduced energy consumptions. Much attention is currently devoted to the study of spin-transfer torque (STT) through which it is possible to realize spontaneous magnetization precession and switching. By using the generation of pure spin currents by ferromagnetic resonance (FMR), spin pumping from a ferromagnet (FM) into a non-magnetic (NM) material is one of the most promising candidates for these applications. Our project aims to the study of the efficacy of spin pumping in perovskite-based iridates thin films and multilayers and the influence of critical parameters as epitaxial strain, interface quality or barrier conductance.

JOB POSITION DESCRIPTION

We are looking for highly motivated candidates with a solid background in physics. The candidate will work in a rich and multidisciplinary environment at the "Advanced Characterization and Nanostructured Materials" (ACNM) group at the Materials Science Institute of Barcelona (ICMAB). The group has a long-standing record of high quality publications in the field of functional oxide materials for novel technologies. Our research is both of basic and applied character since it is aimed not only to investigate the relation between the microstructure and properties but also its potential application for the design and fabrication of novel magnetoelectronic devices. The student will be responsible for the preparation of iridate-based thin films and heterostructures and to perform and analyze magnetodynamic properties.

GROUP LEADER:
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MOLECULAR MATERIALS FOR ELECTRONICS

Design of curcuminoid materials toward the creation of single-molecule hybrid three-terminal devices
Núria Aliaga-Alcalde, Arántzazu González-Campo

RESEARCH PROJECT / RESEARCH GROUP DESCRIPTION

In the last years my group, FunNanoSurf, has developed a family of curcumin derivatives, so-called curcuminoids, CCMoids, applied in the field of Molecular Electronics as nanowires; molecular connectors capable of displaying electron transport through their conjugated bodies in a number of devices that contain electrodes made of gold or graphene and silicon (Si/SiO2). Regarding the molecules, CCmoids are diarylheptanoid systems that contain one -diketone moiety in the central part of the skeleton and aromatic rings on the sides of such conjugated chain.
Now, our goal is the design of new generations of CCMoids that will improve the initial electronic properties found in the past, generating robust final nanodevices. For that, the new CCMoids are going to be designed (i) containing side groups that by covalent attachment within the electrodes (gold, graphene) will provide high conductance values and robust final devices and (ii) the nature of the central conjugated chain will be varied by coordinating different paramagnetic metals to study their effect in the final conductance values and spintronic properties. Finally, break junction technique (BJ) will be used to analyze the outcome of the final systems.
The knowledge amassed in the project will improve the state of the art regarding the creation and understanding of single-molecule nano-devices from the practical and fundamental point of views. The creation of stable nanodevices based on molecules will improve the knowledge gathered in each system, allowing the creation of prototypes and the design of advanced materials in learning-doing cycles.

JOB POSITION DESCRIPTION
The PhD candidate will be trained in (i) organic synthesis toward the characterization of CCMoids; (ii) coordination chemistry, studying different metal centers that could coordinated to the organic moieties and the final coordination compounds achieved; (iii) standard characterization (FT-IR, Mass, Elemental Analysis, Thermogravimetry, 1H NMR, UV-Vis absorbance…) and specialized characterization (electrochemistry, fluorescence, magnetism, x-ray diffraction,…) as well as (iv) techniques to deposit CCMoids (e.g.: soft lithography methods) on a substrates (surfaces, electrodes,…) and the proper analysis of the final systems (AFM, SEM, TEM, contact angle, UV-Vis,…). Finally, the candidate will be trained in (v) electronic measurements of the final devices containing the best molecular candidates (from above, MCBJ-BJ). For that the group has a probe station of six arms that will allow the measurement of the conductance properties as well as additional luminescent features of the final devices or the effect that light can have in them.

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The student will actively participate in group meetings and prepare oral presentations (e.g. group meetings) and writing documents as well as will be responsible of lab duties, sharing them with the other members of the group. He/she will present the final work in workshops and conferences.

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Low-cost and flexible organic electronic devices for bio-sensing
Marta Mas-Torrent

RESEARCH PROJECT / RESEARCH GROUP DESCRIPTION

Due to technological limitations associated with the use of silicon, substantial efforts are currently devoted to developing organic electronics and, in particular, organic field-effect transistors (OFETs). Indeed, the processing characteristics of organic semiconductors make them potentially useful for electronic applications where low-cost, large area coverage and structural flexibility are required.
One important and attractive niche of applications of OFETs is the development of novel low-cost sensing platforms. Particularly, the so-called Electrolyte-Gated Field-Effect Transistors (EGOFETs), which are able to operate in a low voltage window in aqueous medium, have emerged arousing great expectations for the development of biosensors, particularly, for the fabrication of point-of-care (POC) devices.
In this project, we aim at developing novel sensing devices with organic transistors by employing a variety of routes to integrate different bio-receptors. For instance, the recognition agents will be integrated by the functionalisation of the electrodes or in polymeric hydrogel dielectrics. The work will be combined with the optimization and understanding of the materials properties in order to realize stable and reliable devices.
The candidate will have the opportunity to handle a variety of multidisciplinary techniques such as wet chemistry methods, organic materials processing and characterisation, vacuum deposition techniques, laser lithography for electrode fabrication, electrical measurements, morphological and structural characterisation tools, electrochemistry, surface fucntionalisation, etc.

JOB POSITION DESCRIPTION

The candidate will be able to join to a pioneer, dynamic and active group (https://departments.icmab.es/molecularelectronics/) from the Department of Nanoscience and Organic Materials from the Institute of Materials Science of Barcelona (ICMAB-CSIC) (www.icmab.es/nanomol). Our research group is focused on the design and synthesis/preparation of new functional molecular materials for their application in organic/molecular electronic devices. Our work ranges from fundamental studies in order to better understand materials properties to a more applied perspective aiming at developing proof-of-principle devices. Further, the candidate will join a research team which has a long expertise in the field or organic electronics and has actively participated in many European projects in this area.
The candidate will perform the PhD in a very interdisciplinary environment. He/she will be part of a research group composed of chemists, physicists and engineers. For this, the candidate should have the ability to work in a team formed by researchers with different backgrounds and from different nationalities.

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In addition, the successful candidate might travel to other European countries to develop part of the project in the framework of established scientific collaborations or to present the results of his/her research in conferences and schools.
We are looking for highly motivated candidates with excellent academic record. The candidate should hold a Bachelor degree in Chemistry, Physics, or Materials Science and related Master degree.

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Towards a new generation of luminescent boron clusters-organic molecular hybrids for optoelectronic applications
Rosario Núñez

RESEARCH PROJECT / RESEARCH GROUP DESCRIPTION

In the last decade, the development of boron cluster-based organic π-conjugated systems have attracted huge interest as active materials in (opto)electronic devices, such as organic light-emitting diodes (OLEDs), organic field effect transistors (OFETs), solar cells, biological sensors and imaging, among others. One of the challenges has been deciphering the role of boron cluster on the optical and photophysical properties of luminescent materials in solution and solid state.

Owing to our interest in elucidating the influence of boron clusters in the photoluminescent properties of their derivatives and in be able to modulate the fluorescence/phosphorescence efficiency of the systems, in the current project we aim to develop a new generation of boron clusters-organic molecular hybrids as fluorophores of high efficiency and stability to improve the material light-emitting performances. Their completed characterization, including crystal structures established by X-ray diffraction analysis will be performed. Experimental studies regarding photoluminescent properties in solution and solid state will be achieved and complemented with theoretical calculations to establish meaningful structure-photophysical properties relationship for the compounds. Regarding the solid state, it is known that well-defined molecules allow for crystalline materials, in which an adequate design of the molecular structure can lead to the specific intermolecular arrangements needed for optoelectronic properties. One of the major challenges is to establish the structure–property relationships of a specific material, and understand how small changes in the molecular structure might impose large changes in solid state properties.

The candidate will incorporate in the LMI at ICMAB-CSIC. Group's staff members: Prof. Francesc Teixidor, Prof. Clara Viñas, Dr. Rosario Núñez and Dr. Jose Giner-Planas. Our group has leading expertise in boron clusters chemistry and molecular materials, which places us in an ideal position to create innovative applications in materials science, medicine or energy. To date 40 doctors have been graduated and 375 articles published in high impact journals.

JOB POSITION DESCRIPTION

We are looking for good candidates for a PhD position. The project training will give the fellow research unique insights into an approach to do research. The main goal of this project is the design, synthesis, characterization and properties study of new luminescent boron cluster-based

molecular materials with potential optoelectronic applications. For this
purpose, the student will work with air-sensitive compounds to synthesize new building blocks based on boron clusters for their covalent bonding to different fluorophores by using Schlenck techniques (vacuum-nitrogen lines, glovebox). The structural and electronic properties of the boron clusters will play a significant role in the photophysical properties of the final materials. The student will use different spectroscopic techniques for characterization: Infrared Spectroscopy (FT-IR), Nuclear Magnetic Resonance in solution (^{1}H, ^{13}C, ^{11}B-NMR), UV-vis and fluorescence spectroscopy; as well as other useful techniques such as mass spectrometry (MALDI-TOF), DSC-TGA; TEM, SEM among others. This will permit the student to be directly in contact with all these techniques and learn to interpret the spectra and results.

Skill required to applicants: excellent graduates in Chemistry, or Chemical Engineering, with scientific interest and preferably practical training in courses on synthesis, and purification techniques of (chromatography, TLC, recrystallization, sublimation, etc.). Basic knowledge of standard characterization techniques, specially IR and NMR spectroscopy, but also some knowledge of UV-vis and fluorescence spectroscopy, optical microscopy (TEM, SEM), etc. A recently obtained Master of Science level is mandatory.

GROUP LEADER:

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