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GRENOBLE ALPES MÉTROPOLE

	Wednesday, October 23th			Thursday October 24th			Friday October 25th		
8h45				**B1 - Power electronics (Lecture 2)** Jesus Canas Xavier Jordà Yvan Avenas	**A2 - 2D materials for biological applications And energy storage (Amphi)** Cesar Moreno Laura M. Lechuga Thomas Alava	**C3 - Quantum fluids (Mag 2)** Veronica Ahufinger Irenee Frerot Luigi Amico	**D1 - Oxide films - spintronics (Lecture 2)** Josep Fontcuberta Stefania Pizzini Jordi Sort	**D2 : 2D Materials (Amphi)** Hanako Okuno Maciej Jankowski	**D3 - Quantum circuits, quantum thermodynamics and quantum information (Mag 2)** Anna Sanpera Mike Zhitomirsky Pol Forn
10h15				Coffee Break				Coffee break	
10h45				Sergio Busquets David Frey	Cecile Delacour Camille Raillon	Léonie Canet Maxime Richard	Rafael L. Seeger Aliona Nicolenco Gilles Gaudin	Nicolas Rougemaille	Alexia Auffeves Nicolas Roch
11h45				Education round table : Veronica Ahufinger, David Ferrand			Summary and future plans: Jordi Sort, Nicolas Retière, Johann Coraux, Maxime Richard Closing remarks		
12h30				Lunch				Lunch or departure	
14h00	Opening (Amphi) Olivier Buisson Hervé Courtois								
14h30	Anna Sanpera Xavier Obradors Xavier Thibault			**A3 – Semiconductor nanocrystals (Lecture 2)** Andreu Cabot Davina Moodelly	**B2 – Spintronics and heat transport with 2D materials (Amphi)** Juan Sierra Aron Cummings	**C2 - Optical spectroscopy 2D material (Mag 2)** Frank Koppens Laetitia Marty			
15h00	**A1 - Power systems (Lecture 2)** **Jose-Luis Dominguez**	**B3 - Optomechanics (Amphi)** Nadine Meyer	**C1 - Oxide films - materials (Mag 2)**						
15h30	Ramon Costa Castello	Clivia Sotomayor	Jose Santiso Xavier Torrelles	Gerasimos Konstantato	Klaas-Jan Tielrooij	Denis Basko			
16h00	Monica Aragüés Peñalba Xavier Obradors	Jean-Philippe Poizat	Massimiliano Stengel Aude Bailly	Coffee break					
16h30	Coffee break			Anindita Sahoo	Matthieu Jamet	Zeila Zanolli Clément Faugeras			
17h00	Nicolas Retière	Olivier Arcizet	Jean Marc Tonnerre	Peter Reiss					
17h30	Pascal Tixador	Dylan Cattiaux	Fatima Ibrahim	Lab visits					
18h00	Poster session and buffet dinner								
20h00									

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A1 - Power systems

ABSTRACT: CITCEA-UPC

Speaker: Mònica Aragüés Peñalba

Grenoble-Barcelona twin conference : From quantum systems to new materials and smart electrical energy

23-25 Oct 2019 GRENOBLE (France)

Created in 2001, CITCEA-UPC belongs to the Universitat Politècnica de Catalunya (UPC) and it is devoted to research, innovation and technological transfer to the industry. Currently, eight CITCEA-UPC members belong to the staff of professors of UPC and the rest of the team consists of engineers, PhD students and master students, more than sixty people. The group activity is focused on Energy in two big areas: Mechatronics (power electronics) and Enertronics fields. Enertonics is the synergistic combination of power system engineering, smart system engineering, computing and control systems. Besides the research and innovation activities of the center, the professors own a Spin-off company called TeknoCEA that is in charge of transferring research results to the market.

In the enertronics field the competences for the project are:

- Energy management systems design and implementation
- Demand response algorithms and implementation
- Electricity markets and local markets design
- Power system operation
- Renewable energy technology
- Smart Grids
- Electric vehicles integration in power systems
- Power system architecture design
- Storage technology integration in power systems

In the mechatronics field the competences for the project are:

- Power electronics
- Energy resources emulators
- Industrial communications
- Control engineering
- Motor drives

Recent projects where CITCEA has participated will be presented. One of them is RESOLVD H2020, which aims to contribute to setting the next generation of competitive technologies and services for smart grids addressed in the topic LCE-01-2016-2017 (Area: 4- Intelligent electricity distribution grid). The objective is to improve the efficiency and the hosting capacity of distribution networks, in a context of highly distributed renewable generation by introducing flexibility and control in the low voltage grid.

IRI Energy and Fuel Cell Laboratory

Ramon Costa-Castelló
Universitat Politecnica de Catalunya

The Fuel Cells and Energy Systems Laboratory has the goal to develop, validate and test control strategies of energy systems, currently the laboratory focuses in fuel cell based energy conversion systems. The laboratory has six test stations, five of them are provided with oxygen, hydrogen, nitrogen and air inlets in order to work with fuel cells. Each of the five test stations is equipped with the necessary sensors and actuators to work with fuel cells in a safe and automated way, as well as to modify the working conditions that affect a fuel cell (humidity, temperature, flow, etc.). The sixth station is used for special-machines electrical power generation. Depending on the type of experiment, each station is designed with a specific functionality. During the talk, most relevant group capabilities will be described. This capabilities will be illustrated using recent projects.

Answering the Challenges of Future Power Systems

Jose Luis Dominguez-Garcia
Catalonia Institute for Energy Research

The Energetic and electric sector is changing its paradigm, making necessary to adapt the industrial sector to such new model. This change is led by the irruption of the renewable energies, Energy storage, the integration of technologies of information and communication (TIC) and internet, which has provoked the evolution of the classic distribution grid to the Smart Grid, and still continue evolving to the future DigitalGrid. Additionally, several classic static loads have become controllables and new active agents has arisen with the aim of participating on the grid management, as electric vehicles or energy storage systems. These new technologies have provided new capacities (enhanced controllability and observability of the grid, better management, increased flexibility, etc), but also bring new challenges and problems to deal with as power quality, security, coordination, new agents. Thus, new developments are required over all the work fields to ensure the real implementation of such future electrical grids.

In this talk, some of the main challenges imposed by such disruption will be presented, in order to demonstrate the need of interdisciplinarity into smartgrids. It is worth noting that the future of power systems does not belong to only one layer, generation, transmission, distribution or consumption, but to all of them.

G2Elab's power system group research works

Yvon Besanger, Raphaël Caire, Nicolas Retière
Univ. Grenoble Alpes, CNRS, Grenoble INP*, G2Elab, 21 Avenue des Martyrs, Grenoble, 38000, France

It is a time of unprecedented challenges in power systems. We have been facing recently a massive integration of distributed and renewable energy sources, a deregulation of energy markets, growing interactions between power systems' stakeholders, operators, end users and a digitalization of energy systems causing stronger interdependencies between ICT and power systems. Advanced research is required to tackle with the ever increasing complexity of power systems and their necessary smartification to get an electrical system more efficient, more reliable and resilient, more secure.

G2Elab's power system group is the largest academic group working on power systems in France. Its main research direction is about smart networks in the broadest meaning, i.e. from transmission system (e.g. Supergrid) to distribution (smart grids) and embedded systems (e.g. electrical vehicle).It is structured around three themes :

- Non conventional units and systems (electric vehicles, storage units, power converters buildings, data centers…) connected to the grid. They are modelled taking into account user-driver, regulatory or environmental constraints, functional uncertainties, e.g. localization of E.V. at any time. Modeling is used to optimize sizing and power management of stand-alone or networks of units, e.g. micro grids.
- Advanced analysis and optimization of power systems. This theme focus on the optimal design and operation of power systems. Long term planning, over 40 years requires stochastic optimization techniques. Day-ahead or real time management is enabled by new control and reconfiguration functions seeking for the optimal use of network's flexibility resources. Obviously, new planning and operation approaches of power systems co-evolve with energy policies, energy system governance and markets. Game theory and uncertain economy theory are used to better understand how policy and economic practices are entangled and affect the energy system.
- Breakthrough methods for understanding and achieving secure operations of complex infrastructures. Digitalization and smartification of the power systems have increased the interdependencies between critical infrastructures and yield potential major system outage. Understanding vulnerabilities, fault mechanisms, designing monitoring and protection systems are the main objective of this theme, paving the way for future resilient smart grids.

These research works benefit from experimental facilities that are dedicated to the downscale experimention of power systems (i.e. lab microgrids) coupled with power-hardware-in-the-loop (PHIL) real-time simulations.

Some key results and future directions for our research will be presented during the workshop.

* Institute of Engineering Univ. Grenoble Alpes

Advances in processing and applications of high critical current $YBa_2Cu_3O_{7-x}$ coated conductors

X. Obradors

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High temperature superconductors (HTS) are complex oxide quantum materials where nanoscale structural control is required. To fully exploit the novel functional opportunities of these materials a deep understanding of the growth mechanisms is required. A worldwide huge effort in the R&D of HTS high current conductors for large scale power applications and magnets encompasses many materials science and engineering challenges. Coated conductors based on epitaxial $YBa_2Cu_3O_7$ (YBCO) films are one of the most promising alternatives to reach the required performance goals, as well as to reduce the cost down to the levels required to make a reality these technological expectances. In this presentation, several topics related to the recent progress in these HTS nanomaterials will be presented with particular emphasis on the chemical solution deposition (CSD) approach as a bottom-up strategy to reduce the figure of merit cost / performance of the conductors. I will show how colloidal solutions with preformed nanoparticles can lead to enhanced vortex pinning properties. A thorough investigation correlating the pinning landscape with the defect microstructure has been pursuit through HRTEM/STEM analysis. I will also report how CSD nanocomposites can be obtained through a new approach based on a transient-liquid assisted growth (TLAG) enabling ultrafast growth rates in the range of 100 nm/s. Finally, the prospective of using coated conductors to tailor conductors for Fault Current Limiting applications will be also described as an activity derived for the EU project FASTGRID.

This research has been funded by EU-ERC_AdG-2014-669504 ULTRASUPERTAPE project, EU-FP7 NMP-LA-2012-280432 EUROTAPES project, FASTGRID project EU-H2020- 721019 and Excellence Program Severo Ochoa SEV2015-0496.

A2 - 2D materials for biological applications and energy storage

COMBINING NANOPHOTONIC SENSOR PLATFORMS WITH 2D MATERIALS FOR ADVANCED DIAGNOSTICS TOOLS

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Abstract

The need to monitor and detect biological and chemical substances, related to human and environment health in a fast and reliable way, is one of the challenges faced by humanity in the 21st century. Tests done nowadays in laboratories are slow (from several hours to days) and expensive. Modern diagnostics is demanding novel analytical sensing tools that could enable fast, accurate, sensitive, reliable and cost-effective diagnostics.

Photonic biosensors are systems that seize different light-based phenomena for the fast detection and quantification of substances (i.e. toxins or pathogens, whose presence or quantity is an indicator of the onset of a pollution or a disease). Among the different photonic biosensors, Silicon Photonics Biosensors based on evanescent wave sensing principle offer undisputed advantages such as robustness, reliability, high sensitivity and low power consumption. We have introduced a new type of silicon photonic sensor, the bimodal waveguide (BiMW) interferometric biosensor, which is offering an unprecedented sensitivity while operating under a label-free scheme (detection limit of 10^{-8} RIU for bulk sensing and below 0.01 pg.mm^2 for surface sensing). It is also prone to miniaturization and multiplexing as is fabricated in compact silicon nitride waveguides contained on chips.

We have combined this nanophotonic BiMW sensor with MOFs nanoparticles as a synthetic receptor for the selective detection of CO_2. This sensor is constructed via self-assembly of a transparent film of zeolitic imidazolate framework-8 (ZIF-8) nanoparticles (size: 32 ± 5 nm) on the nanowaveguides. The nanoZIF-8-based sensor exhibits a broad linear response, with limit of detections of 3130 ppm at room temperature and 774 ppm at 278 K. Furthermore, it is robust, selective, fast and reusable, and can be stored under humid conditions with no loss in performance.

The unique combination of BiMW sensors with other 2D materials (as graphene nanoribbons) could render in sensing devices with performances behind the state-the-art and we are currently exploring several alternatives.

References

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Graphene SGFET for biosensing : From transductor design to tripod-based non-covalent functionalization

Adrien Hugo,' Juliette Simon[1], Madhav Kumar[1], Riadh Othmen[2], Julien Renard[2], Vincent Bouchiat[2], Chao Sun[5], Jason A. Mann[5], Jeevak M. Parpia[3], Harold G. Craighead[4], William R. Dichtel[5], **Pascal Mailley**[1], Thomas Alava[1]

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The accurate detection of biomarkers for medical diagnosis requires biosensors with high sensitivity and selectivity. Graphene-based Solution-Gated Field-Effect Transistors (SGFET) (**Fig.1.a)**) have shown superior electrical sensitivity in liquid compared to silicon and diamond-based SGFET **[1]**, owing to the outstanding graphene electrical properties. However, selective biosensing requires the introduction of specific bioreceptors at the surface of graphene. Simple adsorption of bioreceptors onto graphene is not suitable, due to irreversible denaturation and / or to lack of orientation of the protein bioreceptor. Besides, covalent grafting of chemical moieties to graphene disrupt its honeycomb lattice, resulting in drastically reduced charge carrier mobility. Aromatic compounds such as pyrene can adsorb onto graphene by π-stacking without deteriorating its properties. Thus, several teams have reported the immobilization of bioreceptors on graphene using pyrene-based spacer molecules **[3]**. Nevertheless, the unambiguous demonstration that such spacers would prevent bioreceptors from denaturation by stacking on graphene, due to a rotational degree of freedom along the spacer carbon chain is still a challenge (**Fig. 1.b)**). In this work, we report the functionalization of graphene SGFET with a tripodal molecule including three pyrene feet (**Fig. 1.c)**).

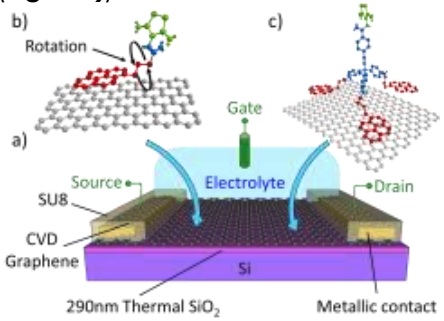

***Figure 1**: a) SGFET, 3D view of b) monovalent pyrene-based spacer and the rotational degree of freedom, c) Tripod with the pyrene feet (red), backbone (blue), reactive ester group (green)*

Such tripodal molecule is 10^3 times more kinetically stable than classical monovalent spacers, and was specifically designed to stably maintain the functional protein bioreceptors away from the graphene surface **[4]**. Micro-fabricated SGFET **[5]** functionalized with the tripod show a reproducible and significant Dirac peak shift. State-of-the-art electrical sensitivity values maintained after tripod immobilization are reported (**Fig.2**). Building upon these promising results, we are currently binding antibodies to the tripod-functionalized SGFET, and assessing the sensitivity of immunological sensing with our biosensors in buffer-engineered media.

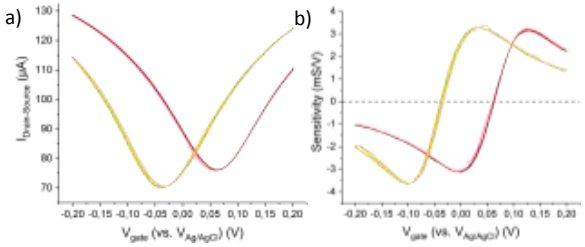

Figure 2: a) Transfer curves and b) sensitivity before (red) and after (yellow) graphene functionalization with the tripod (5 cyclic scans)

References

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From molecules to atomically precise graphene nanoarchitectures

C. Moreno, M. Vilas-Varela,[1] B. Kretz,[2] A. Garcia-Lekue,[2,3] M. V. Costache, M. Paradinas, M. Panighel, M. Tenorio, G. Ceballos, S. O. Valenzuela,[4] D. Peña,[1] and A. Mugarza[4]

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On-surface reactions, via programmed interactions of molecular building blocks, has recently emerged as a promising route to synthesise atomically precise materials from the 'bottom-up'. This approach ensures exquisite atomic-scale control of the structural and chemical functionalization, allowing to design a vast number of carbon-based nanoarchitectures not available by traditional solution chemistry nor with the 'top-down' methodologies. In particular, graphene nanoribbons (GNRs) with different structures can be synthesized with atomic precision and fine-tuned electronic band gap.

In this talk, I will describe the recent advances in the on-surface synthesis field. Then, I will discuss our recent results to synthetize atomically precise nanoporous graphene [1], graphene nanoribbons and their chemical functionalization and how to organize them into superlattices[2,3].

At the end of the day, this talk will demonstrate the full path to synthetize a semiconducting graphene material with a bandgap similar to that of silicon, its atomic-scale characterization, and its implementation in an electronic device. Further potential applications include in photonics and highly selective molecular filtration and sensing systems.

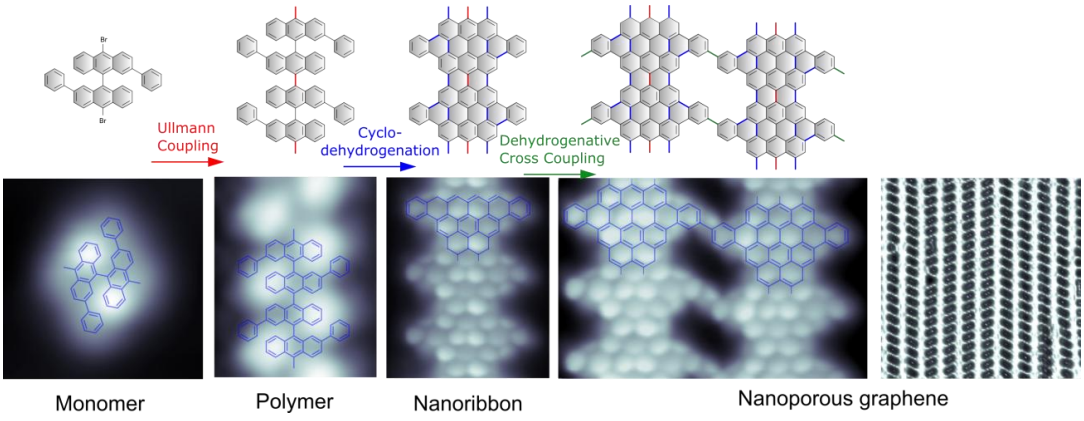

Figure 1. STM images (bottom) and schematic representation (top) of the precursor, intermediates and final product of the hierarchical synthesis of nanoporous graphene.

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[2] C. Moreno; M. Paradinas; M. Vilas-Varela; M. Panighel; G. Ceballos; D. Peña; A. Mugarza. **Chem. Comm.** 54, 9402-9405 (**2018**).

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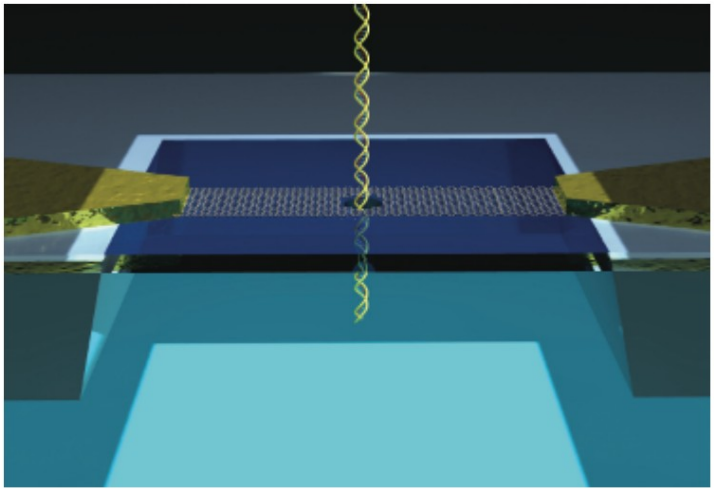
2D materials coupled to nanopores for DNA Sequencing Applications

Camille Raillon
Systèmes Moléculaires et Nanomatériaux pour l'Energie et la Santé (SYMMES)

Today, sequencing technologies are still dominated by methods that require a considerable amount of time in sample preparation to cut and purify DNA into many short copies. This is required to provide adequate signal-to-noise ratios (SNR) for fluorescence-based detection techniques. Direct sequencing of single DNA molecules would eliminate this costly amplification step and enable sequencing of longer strands of DNA, also called Long-Read Sequencing.

In this talk, I will speak about state-of-the art developments that has been done on integrating 2D materials to nanopores [1,2]. For example, graphene nanoribbon integrated to nanopores for the development of a new generation of devices for single-molecule detection and DNA sequencing applications. One of the major advantages of such devices would be to enable long reads of DNA molecules as they translocate through the nanopore.



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Multiscale graphene neuroelectronics

Renato Olarte,[1] Antoine Bourrier,[1] Rhiad Otmen,[1] Anne Briancon-Marjollet,[2] Mireille Albrieux,[3] Gregoire Courtine,[4] Alessandro Cresti,[5] Stephane Roche,[6] Vincent Bouchiat,[1] Cécile Delacour [1]

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2D materials such as graphene offer an ideal platform for recording and culturing neural networks, regarding its exceptional neuronal affinity and the presence of readily accessible surface charges which give the unprecedented possibility to realize a direct electrical coupling with cells. In addition, graphene is highly flexible, optically transparent and could be transferred on a wide range of substrate to be combined with multiple electrophysiological tools.

Here, we will present the cytocompatibility study of pristine monolayer graphene, and its significant advantage for neuroprostheses and *in-vitro* model networks [1]. We will show that the ability to control the neuronal affinity of graphene based neural interface opens the way to a variety of applications such for patterning long-lasting *in-vitro* neural networks, and for brain interfaces to reduce immune response and the glial scars.

Moreover, the nano-structuration of large (mm^2) CVD-grown graphene monolayers allows the fabrication of dense arrays of highly sensitive field effect transistors (G-FETs). Among their successful bio-integrations, the detection of action potentials in numerous electrogenic cells including neurons [2] has paved the road for the high spatio-temporal and wide-field mapping of neuronal activity. We will show that ultimate sensing could also be achieved such the field effect detection of ion channel activity, and will underline the significant contribution of grain boundaries - within the polycrystalline graphene FET channel - which provide highly sensitive sensing sites [3]. Such ultra-sensitive and biocompatible neuroelectronics is highly versatile and should be useful for a wide range of fundamental and applied research areas, including brain-on-chip, pharmacology, and *in-vivo* monitoring or diagnosis.

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A3 - Semiconductor nanocrystals

Infrared Optoelectronics based on Colloidal Quantum Dots

Gerasimos Konstantatos
Institut de Ciencies Fotoniques,
& Institució Catalana de Recerca i Estudis Avançats

Light emission and detection is of paramount importance for a large spectrum of applications. To date, however, current solutions suffer from high costs and lack of CMOS monolithic integration. In this talk I will present recent progress in our lab on high performance infrared solution processed Photodetectors, Light emitting diodes and some preliminary results on stimulated emission based on PbS colloidal quantum dots. Hybrid 2D/CQD photodetectors with record performance will be briefly presented. Then I will present recent results on LEDs with external quantum efficiencies of nearly 8%. I will discuss the use of a ternary colloidal quantum dot blend that has reached this record as a result of electronic passivation of the dots at the suprananocrystalline level. These LEDs have also demonstrated below bandgap turn-on voltage and when operated as solar cells reached open circuit voltages approaching the radiative limit. This has been the result of very low trap state density and reduction of the electronic density of states. In the second part of the talk I will present recent results of doping robustly PbS QDs in the heavy doping regime that has given rise to exciton bleaching and intraband absorption in the mid and long wave infrared. The underlying mechanisms will be discussed followed by the first demonstration of a PbS photodetector sensing light below the bandgap value of bulk PbS and the repercussions of this towards low threshold lasing in an eightfold degerate system such as PbS.

Visible and NIR-emitting silver-based metal chalcogenide quantum dots: promising candidates for biological imaging

Davina Moodelly,[1] Marie Carrière,[1] Peter Reiss[1]

[1] Univ. Grenoble Alpes, CEA, CNRS, Grenoble Institute of Interdisciplinary Research-SyMMES, 38000 Grenoble, France

Colloidal quantum dots (QDs) are an important class of fluorophores for biological applications due to their exceptional optical properties (strong photoluminescence, high resistance against photo-degradation, optical properties tunable with size and composition). Biocompatibility is an essential criterion when considering the use of QDs as biological probes for imaging and biosensing. Ternary cadmium-free quantum dots of the I-III-VI family ($CuInE_2$, $AgInE_2$, E=S,Se) have attracted great attention as alternative candidates since they are inherently non-toxic compared to binary Cd- and Pb-sulfides. In the past 5 years, $AgInS_2$ QDs synthesized both in organic and aqueous media have shown high quantum yields (> 50%) in the visible range (400-700 nm).[1] Due to their enhanced optical properties as compared to more commonly used $CuInS_2$ QDs they have a high potential for biosensing applications such as for example FRET sensors.[2] Their low band gap binary counterpart, Ag_2S QDs, is a good emitter in the NIR range (700-1200 nm). Therefore, it is an interesting candidate for *in vivo* bioimaging as the NIR emission provides higher penetration depths in biological tissues. In this presentation, we will focus on the aqueous synthesis of $AgInS_2$ and Ag_2S QDs (cf. Fig. 1&2). Particular attention will be paid on the discussion of optimization strategies that could be adopted to improve the optical properties of both materials and on the particular photoluminescence mechanisms occurring in these types of QDs.

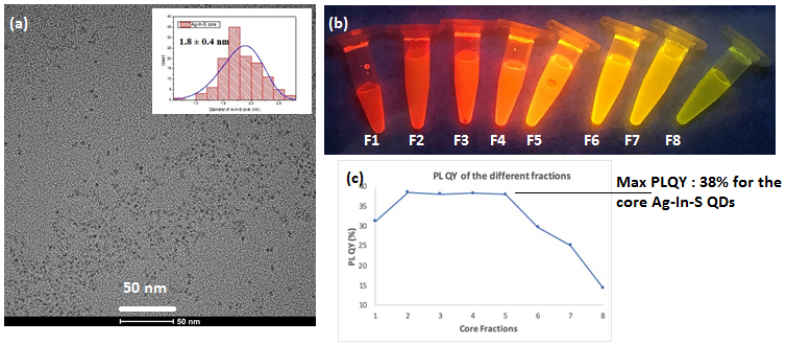

Figure 1: (a) TEM image of $AgInS_2$ QDs prior to size-selective precipitation. (b) Photograph of different size fractions under UV light (365 nm). (c) Evolution of the PLQY of the different fractions.

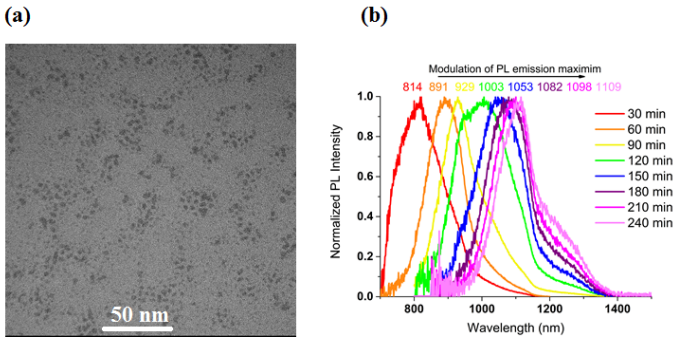

Figure 2: (a) TEM image of Ag_2S QDs synthesized in water. (b) Evolution of the PL spectra as a function of reaction time.

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Ternary semiconductor nanocrystals for energy applications

Peter Reiss

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Semiconductor nanocrystals (NCs), also termed quantum dots (QDs), are characterized by size-dependent optical and electronic properties. Ternary chalcopyrite-type NCs derived from $CuInS_2$ (CIS) are under intense research due to their high potential for replacing Cd- and Pb-based NCs in light emission and energy conversion applications [1]. In contrast to binary QDs (e.g. CdSe, InP), which show narrow band edge photoluminescence with a line width depending on the size distribution, the optical transitions of chalcopyrite-type NCs are governed by intra band gap states. This leads to large effective Stokes shifts and broad emission line widths (both in the range of 200-500 meV) as well as to comparably long PL decay times of several hundreds of nanoseconds [2].

Energy applications like photovoltaics and photocatalysis relying on electron transfer reactions benefit from the flexibility of tuning the electronic properties of chalcopyrite-type NCs with their size and composition. When synthesized in organic solvents, CIS NCs are covered by stabilizing ligands containing long alkyl chains, such as dodecanethiol (DDT). For efficient charge transfer to occur, these long insulating ligands have to be removed from the NC surface and exchanged by smaller molecules or ions. However, this exchange is very inefficient with DDT-capped CIS NCs due to the formation of a compact organic ligand bilayer during synthesis [3]. An interesting alternative approach consists of NC synthesis in aqueous medium. In this case colloidal stability is assured by electrostatic repulsion and therefore very compact stabilizing ligands can be applied. Using this strategy, we optimized the properties of CIS NCs prepared by hydrothermal synthesis for use in quantum dot sensitized solar cells. Aqueous synthesis can also be adapted to generate a thin ZnS shell on the surface of CIS NCs. The obtained core/shell particles have been applied as photo-sensitizers in a hybrid system with a molecular catalyst (Co-complex) to perform photocatalytic hydrogen production in aqueous solution. The developed system exhibits very promising performances, in particular high turnover numbers and an excellent stability are observed [4].

Finally, a brief perspective on another class of emerging luminescent ternary semiconductor nanocrystals – metal halide perovskite nanoparticles – will be given [5]. A novel strategy for stabilizing cubic-phase CsPbX3 NCs (X=Br, I) will be presented implying the use of molecular halogen [6]. CsPbI3 NCs have been successfully integrated into perovskite solar cells with efficiencies exceeding 14%. In the quest for Pb-free metal halide perovskites, CsEuBr3 NCs were explored, which exhibit strong photoluminescence in the deep blue range.

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2D and 0D Nanomaterials based Hybrid Infrared Phototransistor

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In the field of telecommunication, thermal imaging, remote sensing, night assistance car driving etc., the infrared (IR) photodetectors are in high demand. Recently, hybrid phototransistors with highly efficient light absorbing 0D quantum dots and high mobility 2D materials explore a new technology, which dramatically increases the responsivity and gain of the photodetector. Such low dimensional IR phototransistor based on graphene/PbS QD hybrid was first proposed in literature in 2012 [1, 2] till the demonstration in 2017 [3] of a high-resolution broadband image sensor sensitive to ultraviolet, visible and infrared light (300–2000 nm).

In our study, we have investigated the potential of similar hybrid phototransistor and explored the underlying photodetection mechanism in NIR and SWIR regions of optical spectra. We initially studied CVD-grown single layer graphene phototransistor in the NIR region, which showed a responsivity of about 100 A/W, associated with the optical absorption in low–doped Si substrate. Such responsivity is 10^5 orders of magnitude higher [4] than graphene phototransistor on conventional SiO_2/highly-doped Si substrate [5]. In the next step, we synthesized the colloidal PbS QDs absorbing in the NIR as well as SWIR regions and developed a layer-by-layer dip coating with simultaneous ligand exchange procedure in order to deposit homogeneous PbS QD layers on graphene sheet leading to a well fabricated hybrid phototransistor. In the NIR region, we achieved a significantly high responsivity of $\sim 10^7$ A/W at 940 nm with irradiation power density of 13 nW/cm^2. In the SWIR range, similar responsivity of $\sim 10^7$ A/W and a photoconductive gain of about 10^7 have been observed at 1300 nm with irradiation power density of 25 nW/cm^2. Under optimized conditions, we achieved a response time as less as 5 ms.

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From nanocrystals to devices: Strategies to induce crystallographic texture and to increase printing speed

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Bottom-up approaches for producing bulk nanomaterials have traditionally lacked control over the crystallographic alignment of nanograins. This limitation has prevented nanocrystal-based nanomaterials from achieving optimized performances in numerous applications. We demonstrate the production of nanostructured $Bi_xSb_{2-x}Te_3$ and $Bi_2Te_{3-x}Se_x$ alloys with controlled stoichiometry and crystallographic texture through proper selection of the starting building blocks and the adjustment of the nanocrystal-to-nanomaterial consolidation process. In particular, we hot pressed disk-shaped $Bi_xSb_{2-x}Te_3$ and $Bi_2Te_{3-x}Se_x$ nanocrystals and tellurium nanowires as building blocks using multiple pressure and release steps at a temperature above the tellurium melting point. We explain the formation of the textured nanomaterials though a solution-re-precipitation mechanism under a uniaxial pressure. Additionally, we further demonstrate these alloys to reach unprecedented thermoelectric figures of merit, up to ZT=1.96 at 420 K, with an average value of ZT_{ave}=1.77 for the record material in the temperature range 320-500 K, thus potentially allowing up to 60 % higher energy conversion efficiencies than commercial materials. Besides, I will also present our results on a new high resolution and ultrafast 3D printing strategy based on electrohydrodynamic jetting.

B1 - Power electronics

G2Elab latest research works in the field of power semiconductor implementation

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Wide bandgap semiconductor materials (WBG) have open possibilities for performance and technological breakthroughs. By using them, it is theoretically possible to increase switching frequency while reducing losses, to manufacture more compact converters and to implement them in applications with higher ambient temperatures environments and/or higher voltages. However, their implementation remains a major issue because of the following constraints:

- Increasing the switching speed of devices causes overvoltage at turn-off due to switching cell stray inductance and higher common mode currents due to stray capacitances. Therefore, they cause electromagnetic disturbances (conducted and radiated) more than classical silicon components and then impact the design of gate driver circuits.
- The dielectric field strength of WBG power devices is larger, their working temperature and power density are also increased. The materials and circuits surrounding the power dies are therefore to be adapted to these constraints.

On one hand, the research carried out at G2Elab is proposing several innovating solutions for improving the use of WBG semiconductors. In this context, new architectures of cascaded gate drive circuits are proposed and evaluated in different conditions, series-connected semiconductor devices for example. New power module structures, based on the power chip-on-chip implementation method, are proposed to reduce the electromagnetic disturbances. Today, the main work on power modules deals with the design of ultra low stray inductance power modules while optimizing the global EMC signature and the thermal behavior.

On the other hand, several works are carried out on the implementation and characterization of new materials and devices. The aging and performances of high temperature isolation materials (elastomers and liquids) as well as die attaches are evaluated. Last but not least, diamond devices manufactured by Institut Néel are modeled and characterized under static and dynamic conditions.

Power Converter Design Based on Switching-Cell Arrays

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– *Abstract*:

Power Electronics is a fundamental and ubiquitous technology. The traditional design approach of power converters involves a range of power semiconductor devices with different voltage/current ratings, optimized to operate at different conditions, where different suitable ancillary circuitry and power circuit topologies are also required. This dispersion in power devices and circuits leads to significant engineering efforts, the inability to take full advantage from scale economies to reduce costs, and the inability to concentrate efforts to improve performance. To overcome these limitations, this presentation proposes the introduction of a new configurable device consisting on a matrix arrangement of switching cells, each cell formed by a single power transistor with antiparallel diode, at a single voltage rating, plus ancillary circuitry. By properly interconnecting the switching cells, this novel device can be used as a building block to implement any desired type of power conversion (dc-dc, dc-ac, ac-ac) at a wide voltage and current rating range. Engineering efforts can be then focused on optimizing the specific basic cell. In addition, the design of power converters based on these switching-cell arrays inherently implies the use of multilevel structures, with additional performance benefits, both at the power converter and system level.

The proposed novel configurable power electronic device is only formed by an array of switching cells with no bulky passive components, and a suitable control allows the distribution of power losses through the structure. Therefore, it has a potential to be highly integrated, leading to a very compact implementation.

The introduction of this new power device aims to enable and promote a paradigm shift in the design of power converters that leads to a higher degree of standardization, lower design and implementation costs, increased power density, and superior converter and system performance.

Silicon dioxide MOS capacitors on (100) p- diamond

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Diamond is expected to become the ultimate semiconductor for high power devices due to its superior physical properties such as high breakdown field, low dielectric constant, high carrier mobility or high thermal conductivity. However, the fabrication of an adequate diamond MOS capacitor structure is one of the bottlenecks for the fabrication of a diamond MOSFET. In contrast to the Si technology, where the gate dielectric is a thin layer of silicon dioxide grown by thermal annealing, gate oxides for diamond technology are usually grown by atomic layer deposition (ALD). Alumina, Hafnia or Zirconia are the most studied oxides to fabricate the gate of a diamond MOSFET, but they usually display leakage currents, high interfacial states leading to fermi level pinning, or capacitance-frequency dependence.

Thanks to the recent advances in the ALD deposition of silicon dioxide, the behavior of this gate oxide can be evaluated for first time in diamond MOS capacitor structures. In the present contribution, the characteristics of a silicon dioxide MOS capacitor fabricated on (100) oriented p type diamond are presented. The device has been evaluated thanks to C(V) and C(f) measurements and transmission electron microscopy (TEM) measurements. The capacitor shows both accumulation and deep depletion regimes. Detailed analysis of the device characteristics reveals no leakage currents, low interface states and no frequency dependence of the capacitance. These promising results open the route for the fabrication of a diamond MOSFET with a silicon dioxide gate.

Workshop Lanef – Barcelone

Title: Power electronics based multiscale conversion systems: design and optimization

Presenter: David FREY (G2Elab)

The power transfer using electrical power is almost generalized in all applications. The efficiency of power distribution and grid stability are major issues of this new electrical revolution. Both smart grids, with the massive insertion of intermittent renewable sources, and embedded grids are under concern.

To face this challenge, power electronics converters are very attractive solutions, due to high efficiency. Several topologies are available to increase the power processing, and the latest development exhibit very complex structures, which can only work in closed loop, associated with a very powerful control. However, if centralized converters can be attractive, distributed & communicant systems may also be interesting, since they can offer overall better efficiency, by processing the power at the right place. Stability issues can nevertheless be encountered in this distributed configuration, what is less the case of single point conversion.

To offer the best efficiency, a first task is to be able to optimize the converter, taking into consideration both technological constraints and system level requirements. The method will be introduced in the first part of the presentation.

In a second part, a promising structure for distributed power electronics will be presented, based on a multiple active Bridge topology. The various degrees of freedom of this structure offers a lot of possibilities to optimize both the converter behavior and the system level.

Future work will have to address the system level optimization and will allow choosing the best trade off among centralized, semi centralized or distributed system of conversion.

Semiconductor Power Devices, Technologies and Systems at IMB-CNM

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The Power Devices and Systems Group (PDSG) of IMB-CNM was established in 1985. Its activity focuses on the design, fabrication, characterization and integration of power semiconductor devices, optimized for developing reliable and energy efficient converters and electronic systems, operating even in harsh environments (high temperature, radioactive environments, etc.). The devices developed by the PDSG on different semiconductors (Si, SiC, GaN, diamond), are fabricated in the Clean Room of IMB-CNM and cover various application fields (traction, protection, high frequency, space, high energy physics, etc.). The research work of the Group also aims to transfer the developed technology to the national and international industry sector. The Group's objectives are addressed into three main research lines:

(1) **Silicon Power Devices**: The objective of this research line is developing new Si semiconcuctor fabrication technologies required in advanced power devices such as smart 6.5 kV IGBTs with monolithically integrated voltage and current sensors, super-junction MOS transistors for or 3.3 kV MOS-controlled thyristor structures for smart power distribution networks. The effect of ionizing radiation on power devices to optimize their operation in radioactive environments has also been studied, as well as their usde as radiation detectors. In this framework, new high gain diodes in 2D and 3D configuration for use in future accelerator detectors (ILC) have been also designed and manufactured.

(2) **Wide Bandgap Semiconductor Devices**. The main objectives of this research line are: i) Development of individual steps and optimized process technologies for wide bandgap semiconductors (mainly SiC, and also GaN, diamond, GaO). ii) Design, fabrication and characterization of new power devices based on these materials for high-voltage and high temperature applications. In SiC, we focused especially on gate-controlled MOS structures, JFET devices and very high voltage diodes (> 5kV). These devices are required for renewable energy applications, railway transport and energy distribution. In GaN, we worked on MIS-HEMT devices for the 600V application range, such as electric car and power supplies. iii) Fabrication of high-temperature devices (diodes, switches, integrated circuits) for aeronautical and space applications. iv) The above activities are complemented with the study of carbon-based materials as, for example, epitaxial graphene on SiC or carbon nanotubes.

(3) **Power Systems Integration and Reliability**: The main goal of this research line is the development of technologies to improve the levels of integration in power electronic systems, and the study of the physical phenomena allowing their implementation. Specifically, the activity focuses on four fields. i) Thermal Management: Thermal design, simulation, modelling, characterization and parameter identification of power modules. ii) Power Packaging: Design and development of advanced power modules and assembly technologies. iii) Electro-Thermal Characterization: Development of advanced thermographic systems based on optical and infrared methods for accurate electro-thermal characterization at chip and system level. iv) Reliability: New methodologies for the analysis of the operation limits and reliability of power devices.

B2 - Spintronics and heat transport with 2D materials

Simulation of charge and spin transport in disordered low-dimensional materials

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In this talk, I will present an overview of the Theoretical and Computational Nanoscience Group's work on simulations of charge and spin transport in large-area disordered low-dimensional materials. I will discuss a variety of studies, including the electronic, thermoelectric, and spintronic properties of polycrystalline graphene; spin transport and spin-to-charge conversion in graphene interfaced with high-spin-orbit materials; the performance of graphene-based gas sensors; characterization of graphene oxides; and device simulations testing the limits of conventional spin transport theory. I will also introduce some future areas of interest for the group, including simulations of spin torque for memory applications; and coupling of optical, electronic, and vibrational degrees of freedom for energy harvesting or conversion applications.

Van der Waals epitaxy of transition metal dichalcogenides by MBE Application to the study of the valley Nernst effect in WSe_2

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In this presentation, I will first review our recent results on the MBE growth of transition metal dichalcogenides on various substrates over large areas and explain the mechanisms underlying the van der Waals epitaxy regime. Using this growth technique, we could study the interplay between thermoelectricity and the valley degree of freedom in monolayers of WSe_2. For this purpose, high quality WSe_2 mono and multilayers were grown on epitaxial graphene on SiC. Using millimeter-sized samples, we were able to apply well-defined temperature gradients and demonstrate the very strong Seebeck response of this material. In a second step, we used the ferromagnetic resonance-spin pumping technique to (i) apply the temperature gradient by off centering the sample in the radio frequency (RF) cavity and (ii) address a single valley using the spin pumping through spin-valley coupling. The combination of a temperature gradient and the valley polarization lead to the valley Nernst effect in WSe_2 that we could detect electrically in the RF cavity. The Nernst coefficient we measured is in very good agreement with the predicted value. This effect could be exploited to generate large transverse valley currents for valleytronics applications.

Spin-orbit and spin-heat interaction in graphene lateral devices

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In recent years, spin-based technologies, in which information is carried by spin instead of charge, have become promising for "beyond-CMOS" devices. Graphene and other two-dimensional materials have rapidly established themselves as intriguing building blocks for spintronics applications [1]. Owing to graphene intrinsic low spin-orbit interaction, spins can flow snugly through its crystal lattice over long distances resulting in an ideal spin channel but, at the same time, making it difficult to manipulate spins, which is the cornerstone for successfully implementing spin-based devices. In this talk I will first present a series of experiments where we study spin transport and relaxation mechanisms in graphene/transition-metal dichalcogenide van der Waals heterostructures [2]. I will show how modification of the graphene spin-orbit interaction by proximity effect results in anisotropic spin dynamics and how this finding is essential for spin-to charge conversion on these layered systems [3]. In the second part of the talk, I will discuss the interaction of spin and heat currents in graphene and how spin propagation can be reinforced by the presence of thermal gradients [4, 5].

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Ultrafast dynamics of charge and heat in 2D materials – K.J. Tielrooij, ICN2

With an interest in both fundamental physics and potential technological applications, we study transport of charges and heat in 2D materials. In one of our preferred techniques, we employ ultrafast (sub-picosecond) laser pulses to understand the heating-cooling dynamics of electrons in graphene, and how photocurrent is generated [1]. This understanding has recently led to the development of sensitive and very fast detectors of terahertz light [2] and the efficient creation of terahertz harmonics [3]. Currently, we are studying the spatiotemporal dynamics of charges, excitons and heat in 2D materials, where we have observed promising results that include a peculiar phenomenon that so far has not been reported at room temperature [4].

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B3 - Optomechanics

Cooling levitated nanoparticles in a high finesse cavity

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A few decades ago laser cooling techniques revolutionised many atomic-scale systems, enabling the study of trapped ions and the generation of Bose –Einstein condensates but despite its unprecedented success an atomic resonance is always needed. In the context of cavity optomechanics alternative techniques without the need of atomic resonances have widened this possibility towards the cooling of macroscopic objects[1]. Recently the radiation pressure cooling of mechanical oscillators [2], optomechanically induced transparency [3] and ground state cooling [4, 5] have been demonstrated.
Current progress in optomechanics has brought forward multiple experimental platforms [6, 7] of which many platforms necessitate complex cryogenic environments and suffer from clamping losses as major decoherence sources. An alternative approach is the cooling of levitated nanoparticles from room temperature, which have been suggested for probing quantum mechanics on the mesoscopic scale [8, 9]. In levitated systems collisions with residual gas molecules and photon recoil heating are now the remaining decoherence sources [10] opening the way towards low phonon occupations. In the context of cavity optomechanics, resolved sideband cooling of a levitated nanoparticle has recently been realised [11, 12].
Here we demonstrate the resolved sideband cooling of a levitated nanoparticle within a high finesse cavity at high vacuum. Trapping the nanoparticle in an external optical tweezer allows on one hand the free positioning of the particle within the cavity field and on the other hand the additional cooling via parametric feedback cooling [13]. The combination with well-established resolved sideband cooling techniques creates a powerful platform for controlling the centre of mass motion (COM) of a mesoscopic object. By exploiting cavity enhanced Anti-Stokes scattering we all optically cool the COM to minimum temperatures of $T \approx 10mK$ for a silica particle of 235nm diameter. Power dependent phase noise heating is observed, being the main current limitation in reaching lower temperatures. In the future phase noise suppression for resolved side band cooling brings low phonon occupation numbers of mesoscopic systems via passive cooling schemes within the reach of table top experiments at room temperatures.

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Micro-engine driven by a single quantum dot

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In this work, we use an hybrid system, made of a vibrating wire of mass ~1 ng and a semi-conductor quantum dot (QD) coupled via strain. A few years ago, some of us have shown that the energy of the QD depends on the strain generated by the wire oscillations [1]. We demonstrate here the reverse effect [2], whereby the wire is set in oscillation by the resonant drive of the QD by a laser modulated at the mechanical frequency (400 kHz). This realizes an engine powered via a single quantum system, and from a more fundamental point of view, this opens the way for the realization of quantum states of motion with the transfer of the « quantumness » of a two-level system towards a macroscopic mechanical oscillator.

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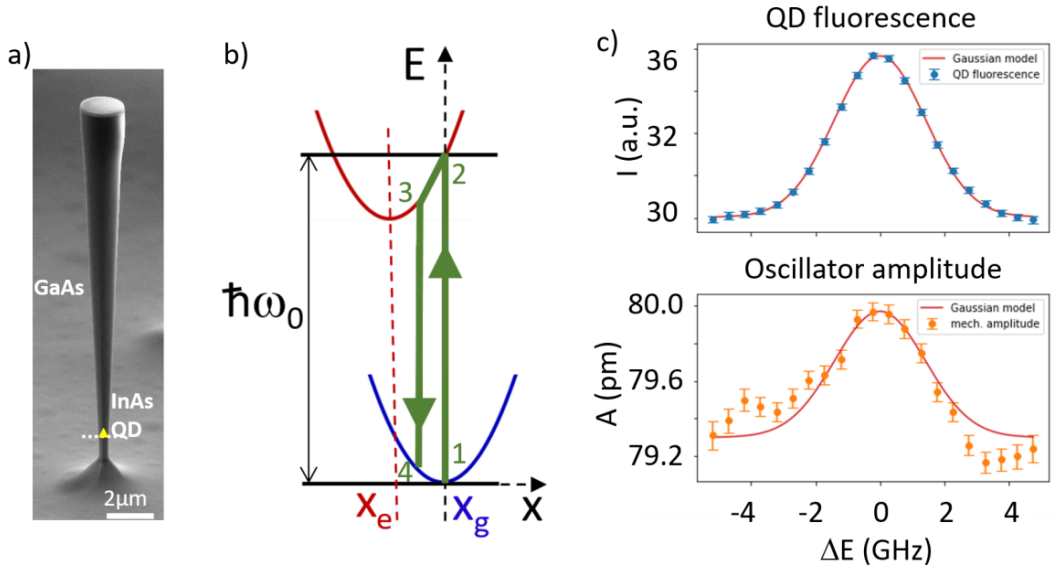

Figure 1 : (a) Scanning electronic microscope image of the photonic wire. b) When the QD is excited, the rest position of the mechanical oscillator is shifted by x_g-x_e=(g/Ω)x_{zpf}. c)Top, fluorescence light emitted by the QD, and, bottom, motion amplitude of the wire, as the laser is scanned across the QD resonance.

TOWARDS PHONON CIRCUITS BASED ON OPTOMECHANICS*

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Optomechanical (OM) elements are designed by overlapping optical and mechanical modes in confined volumes, e.g. nanobeam cavities, in which the room temperature mechanical quality factors have been shown to reach > 10^3. We previously demonstrated a coherent phonon emitter at 0.3 GHz via self-pulsing [1] and up to 5 GHz via dynamical back-action [2]. The silicon OM nanobeam is the key element in our strategy towards phononic circuits. The nanobeam is coupled evanescently via a tapered fibre either directly to the OM cavity or to an integrated photonic waveguide. The non-linear interactions can be controlled to reach a chaotic regime[3], and with an external laser, the coherent phonon emission can be modulated [4].
To realise a phononic circuit, several elements fulfilling different functions have to be integrated. For example, a mechanical tether is used to link two nominally identical OM nanobeams and show that the mechanical signal from one cavity be detected in the other cavity and that cavities synchronize their oscillations under specific conditions [5]. This synchronised state, in the form of a "master-slave" synchronisation, could be used as a clock in integrated phononic circuits and can be modulated in the same way as individual cavities. Preliminary experiments to integrate a waveguide have been carried out and showed that a photonic waveguide can be used to couple light in and out of the cavities and to observe phonon lasing, thus paving the way to more complex phononic circuits with multiple cavities addressed from a single entry point on the phononic chip.

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Nonlinear self-induced oscillations in microwave optomechanics

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We report on self-sustained oscillations studied on geometrically different mechanical devices embedded in a microwave optomechanical setup. A strong blue-detuned pump signal (at a frequency shifted up from the cavity by the mechanical frequency) triggers the parametric instability. Two different NEMS (Nano-Electro-Mechanical Systems) dynamics are compared: the ones of a doubly-clamped beam [1] and of a drumhead [2]. Measurements have been carried out from 1 K down to 10 mK for different applied microwave powers and detunings. The drum device displays much less hysteretic behavior than the beam, and the detected amplitude signal for the drum is more than 1 order of magnitude larger than for the beam. Nonlinearities (of different strengths or nature) in these systems seem to be the key to understand these facts. We analyze the results in the framework of an extended optomechanical theory including Duffing-type and coupling nonlinear terms. Quantitative understanding of this regime should enable its use as a new resource for microwave electronic circuits.

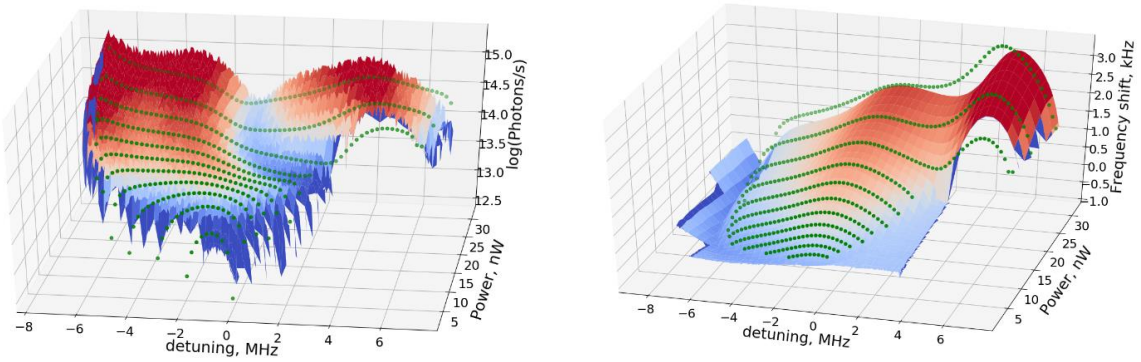

Figure 1: Left: Equivalent output photon flux at 210 mK: Experimental data (Colormap) and numerical simulation (green points) with g_0=10 Hz, g_1=1e-7g_0, g_2=-1e-13g_0 and γ_m=350 Hz. Right: Frequency shift of the self-oscillation peak at 210 mK: Numerical simulation (green points) with g_0=10 Hz, g_1=1e-7g_0, g_2=-1e-13g_0 and γ_m=350 Hz and the fitted normalized duffing parameter β=240 Hz.

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C1 - Magnetism/oxide films 1: materials, elaboration, structure

Structural investigation during the metal-insulator transition of an epitaxial VO_2 film

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Bulk vanadium dioxide (VO_2) exhibits a first-order insulator-metal transition (IMT) at T_{IMT} ~ 68°C. During this transition, the VO_2 structure evolves from the monoclinic M1 phase at room temperature (RT) to the tetragonal (rutile R) phase above T_{IMT}, while the resistivity drastically decreases by several orders of magnitude. The changes in the electrical and optical properties make VO_2 a potential material for integration in energy-related devices. The VO_2 IMT characteristics can be tuned by chemical doping and/or strain engineering and metastable phases may occasionally appear; making mandatory *in situ* temperature-dependent measurements. We hereby present a structural study performed during the IMT of a 420 nm-thick VO_2 film epitaxially grown on Al_2O_3 (0001). We took advantage of the complementarity between high-resolution X-ray diffraction and Raman spectroscopy to address the crystallographic phases present during the IMT and their respective temperature range of existence[1]. Three different polymorphs of VO_2 turn out to be involved in the transition: the M1 and the rutile-like R phases are encountered, respectively at RT and above T_{IMT}. The third polymorph, evidenced close to T_{IMT}, is similar to the monoclinic M2 phase. The different depth scales probed by the two techniques suggest that the M2 polymorph would be likely present at the interface. We introduce two structural models accounting for the possible in-plane epitaxial relationships of the film. These models imply a 2 or 4% tensile strain along the in-plane epitaxial direction. For the film studied here, the 2% strain does not drastically affect the transition temperature, as it is found to be close to the bulk value.

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Spin-orbit induced phenomena at ferromagnet/oxide and ferromagnet/2D material interfaces from first principles

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Spin-orbit coupling (SOC) at material interfaces leads to the emergence of a wealth of phenomena such as perpendicular magnetic anisotropy (PMA) and Dzyaloshinskii–Moriya interaction (DMI). Magnetic tunnel junctions based on Co(Fe)/oxide and Co/graphene interfaces have attracted much attention due to their low spin-orbit coupling but yet interesting magnetic and spin-orbitronic properties [1,2]. Using first-principles calculations, we investigate both PMA and DMI emerging at such interfaces. In the first part of the talk, the underlying mechanisms of PMA and its voltage control (VCMA) at Fe/MgO interfaces are discussed. Namely, we distinguish between charge-mediated [3] and ionic-migration [4] induced VCMA which lead to substantially different strengths of the effect. Based on our findings, one can distinguish the driving mechanism from the order of magnitude of the VCMA. In the second part, the PMA and DMI at Co/2-dimensional material interfaces are addressed, where we demonstrate a large PMA and DMI at Co/graphene and Co/h-BN interfaces [5,6]. The significant DMI at such interfaces rises from the presence of Rashba effect which in turn emerges from the intrinsic dipole at the interface.

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Strain-engineered microstructures in epitaxial thin oxide films

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During epitaxial growth complex oxide films may show a variety of competing strain release mechanisms in order to accommodate the mismatch with the substrate, such as misfit dislocation generation, domain formation or even surface topography modifications. This may depend on the magnitude of the cell parameters difference, whether it is compressive or tensile, film thickness, as well as growth rate. The different way films release the epitaxial stress may result in a completely different microstructure, which in turns could have an impact in their functional properties. In this work we show some examples of how classical La0.7Sr0.3MnO3 (LSMO) and VO2 epitaxial films could result in different microstructures depending on the strain release mechanism. In the first example archetypical rhombohedral LSMO with perovskite structure grown on cubic SrTiO3 substrates is submitted to a slight tensile strain (below +1%). It adopts a highly coherent structure with no apparent misfit dislocations. The films show clear twin domains with well-developed [100]/[010] twin walls self-arranged in a perfect striped structure [1,2]. However, the same type of film material deposited under higher growth rate conditions develops some surface instability that tends to result in surface corrugation, creating local depressions and forming a distributed array of deep pits of about 10-40 nm lateral size [3-5]. A very different situation is observed when growing LSMO under similar conditions on LaAlO3 substrates, with -2% compressive mismatch. In this case, the films tend to relax from early stages by generating misfit dislocations running parallel to [100]/[010] forming a perfectly arranged crossed pattern. A close inspection of film microstructure reveals that it consists of distinct phases at a nanometric scale inside and around the dislocation cores. [6-8]. In a second example, we show how microstructure of epitaxial VO2 films deposited on TiO2(001) substrates changes during metal-insulator transition slightly above room temperature. Upon cooling down films reveal a progressive variation in the coexistence of lowtemperature distorted monoclinic and high-temperature tetragonal rutile domains, which ultimately generate very large local stresses resulting in film microcracks. This large variety of film microstructures in LSMO and VO2 are phenomenological examples of how complex may be the control over film microstructure in materials with metal-oxide octahedral framework structures, but at the same time how powerful could be the strain-engineering over these materials.

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First-principles theory of flexoelectricity and related materials properties

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Flexoelectricity, describing the polarization response to a gradient of the strain, is a universal property of all insulators that has attracted considerable attention in the past few years. [1] In spite of its fundamental and practical interest, it has long resisted theoretical attempts at quantifying it with predictive accuracy in realistic materials. In this talk, I will introduce the methodological advances that have recently lifted this limitation in the context of firstprinciples electronic-structure theory. [2] I will discuss applications to perovskite-structure SrTiO3, either in the cubic [3] or ferroelastic tetragonal phase. [4] I will also emphasize the generality of these newly established theoretical tools, with interesting connections to the physics of orbital magnetism, natural optical activity and magnetoelectric couplings.

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Depth resolved magnetism in heterostructures of ultrathin films studied by soft x-ray resonant reflectivity

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Heterostructures, based on the stack of ultrathin films with different magnetic states, are nowadays intensively studied, particularly in the context of nanomagnetism and spintronics. The size reduction increases the role of interfaces and couplings at interfaces or through spacing layers. The determination of the magnetization profile, with a sub-nanometer spatial resolution, and modifications that occur at buried interfaces is an important challenge in order to contribute to the understanding of the properties of these systems and their behavior under the influence of various parameters.

Polarized x-ray resonant magnetic reflectivity (XRMR) is now a well-established technique that combines the depth-resolved information of x-ray reflectivity with the chemical selectivity of x-ray magnetic circular dichroism for probing the magnetization profile in thin films and multilayers. Because of the dependence of the atomic scattering factor or of the refraction index with respect to the incoming photon energy, scattering-vector, and polarization state of the incident and reflected beam, XRMR is a unique tool to investigate magnetic ordering and magnetic moments orientation with element specificity.

The capabilities of XRMR in the soft x-ray range will be illustrated through examples focusing on oxide materials.

Structural reconstructions of the polar (111) SrTiO3 surface

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ABSTRACT

Polar surfaces are known to be unstable due to the divergence of the surface electrostatic energy. In this talk the experimental determination of the surface structure of polar Ti-terminated (111) $SrTiO_3$ single crystals by grazing incidence x-ray diffraction is reported. The polar instability of the 1 × 1 surface is solved by a pure electronic reconstruction mechanism, which induces out-of-plane ionic displacements typical of the polar response of $SrTiO_3$ layers to an electron confining potential. On the other hand, the surface instability can be also eliminated by a structural reconstruction driven by a change in the surface stoichiometry, which induces a variety of 3 × 3 (111) $SrTiO_3$ surfaces consisting in an incomplete Ti (surface)–O_2 (subsurface) layer covering the 1 × 1 Ti-terminated (111) $SrTiO_3$ truncated crystal. In both cases, the TiO_6 octahedra are characterized by trigonal distortions affecting the structural and the electronic symmetry of several unit cells from the surface. These findings show that the stabilization of the polar (111) $SrTiO_3$ surface can lead to the formation of quasitwo- dimensional electron systems characterized by radically different ground states which depend on the surface reconstructions.

C2 - Optical spectroscopy 2D material

Photoluminescence of graphene quantum dots: the role of chiral symmetry

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We analyse the electronic and optical properties of graphene quantum dots (GQD) using accurate *ab initio* many-body *GW* and Bethe-Salpeter calculations. We show that most pristine GQD, including structures with irregular shapes, are characterized by low energy dark singlet excitations that quench fluorescence. We rationalize this property by exploiting the chiral symmetry of low energy electronic states in graphitic systems. Edge functional groups with sp^3 bonding are consistently shown to efficiently brighten these low lying excitations by distorting the sp^2 backbone planar symmetry. Such findings reveal an original indirect scenario for the influence of functionalization on the photoluminescence properties.

Dark and Bright excitons in heterostructures of 2D semiconductors

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Monolayers of semiconducting transition metal dichalcogenides are direct band gap semiconductors for which the direct band gap is located in the two inequivalent K and K' valleys. Because of the lack of inversion symetry and of the large spin orbit interaction, the spin and valley degrees of freedom are strongly coupled and a particular valley exciton population can be initialized using circularly polarized light excitation. As two dimensional materials, monolayers can be stacked on top of one another in the form of van der waals heterostructures to create artifical hetero- or homo- bilayers. These artifical structures can host different types of exciton complexes, in particular interlayer excitons for which electrons and holes are in different layers. Recently, it was realized that the twist angle between the two layers can strongly modify the electronic properties of the stack and can also be used to generate a lateral modulation of the potential through a moiré pattern.

In this talk, I will describe optical properties of bright and dark excitons in monolayers of TMD encapsulated in hexagonal boron nitride. Dark excitons are activated by magnetic fields applied in different configurations. The exchange interaction mixes dark excitons in the two valleys and I will show how this mixing can be monitored by external magbetic fields. In a second part, I will describe optical properties of a WSe2/MoSe2 heterobilayer in which the two layers have been aligned with an angle close to 60° (2H stacking) to create a well defined band structure together with a moiré potential. I will show how these particular structures, combined with the use of high magnetic fields, allow for a rich spectroscopy of interlayer exciton scattering mechanisms.

Strong influence on 2D materials of substrate and defects revealed by optical and vibrational spectroscopies

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Atomically thin materials in 2D are attracting much interest since reduction of dimensionality strongly modifies their properties and provides a playground to revisit physical phenomena at the nanoscale. The possibility to exfoliate lamellar materials down to the single layer has provided a wealth of 2D materials with a wide range of physical properties. However, as surfaces with no bulk, these materials are extremely sensitive to their environment.

In particular, the substrate used to support the 2D materials turns as a key factor to determine the system overall physical properties. First, the textbook case of graphene is presented, for which vibrational spectroscopy is a very efficient and non-invasive probe. Our studies highlight the dramatic influence of the substrate on doping and strain [1]. We therefore aim at reducing the influence of the substrate and investigate the specific case of graphene membranes, and in particular, spatial distribution of strain in them [2]. Last, in the case of a non-invasive substrate such as h-BN, intrinsic defects and impurities come into play. Combined spectroscopies, such as photoluminescence and Raman diffusion, provide insights into the nature of defects and their influence on light emission [3].

In the field of 2D materials, optical spectroscopies turn out as very valuable tools to address the delicate question of “intrinsic” optical and electronic properties of atomically thin materials.

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Author: Zeila Zanolli

Title: Ab initio exciton and phonon dynamics in Transition Metal Dichalcogenides"

Abstract:

The interest in the properties of transition metal dichalcogenides (TMDs) has increased due to the discovery of the coupling between spin and valley degrees of freedom, which can be seen experimentally using a circularly polarised laser. After excitation the newly formed carrier populations must move towards the other valley until balance is reached. However, this relaxation process is not entirely understood in the literature, where the relative importance of the electron-electron (e-e) or electron-phonon (e-p) interactions is still a subject of debate. Previous works on WSe_2 [A. Molina-Sánchez, et al. Nano letters 17, 4549 (2017)] have shown that the e-p interaction is a good candidate to describe the relaxation process. Using a fully ab-initio framework based on the Baym-Kadanoff equations [P. M. M. C. de Melo and A. Marini, Phys. Rev. B 93, 155102 (2016)] we study the influence of the e-p interaction on MoSe_2 after its excitation by a laser field. We show how phonons allow carrier relaxation and how the Kerr signal and total magnetisation are affected at different temperatures, with the latter exhibiting a non-monotonic behaviour as the temperature increases [M. Ersfeld et al. Nano Lett. 19, 4083 (2019)].

Nanoscale optics of twisted 2D materials

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Moiré patterns are well-known phenomena in art, textiles and mathematics, which originate from the overlay of two periodic patterns. Intriguingly, atomically thin materials can be stacked on top of each other such that a new periodic pattern can emerge: the moiré superlattice. This can result in a dramatic modification of the electronic and optical properties of twisted 2D materials, compared to those of a single layer. The moiré superlattice can give rise to a plethora of interesting phenomena such as topological bands [1] and many-body phases like superconductivity and magnetism.

A tantalizing example is twisted bilayer graphene near the magic angle (MABG), which exhibits flat superlattice minibands, effectively localizing electrons in a periodic lattice with a period of about 15 nm. Several strongly correlated phases have been observed, including superconductivity and the Mott-like insulating state [2].

In this talk, we give an overview of the nano-optical properties of stacked and twisted 2D materials. Nanoscale optical techniques such as near-field optical microscopy reveal unique observations of strongly confined propagating optical fields, topological domain wall boundaries, and a different type of collective modes in charge neutral TBG near the magic angle [3].

The freedom to engineer these so-called optical and electronic quantum metamaterials [4] is expected to expose a myriad of unexpected phenomena.

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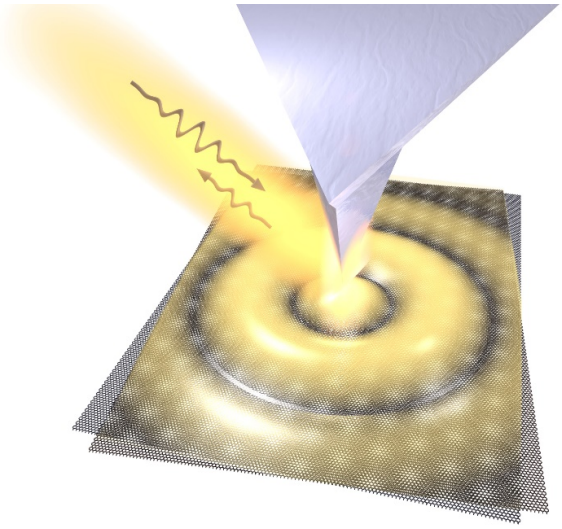

C3 - Quantum fluids and gases

Topology and quantum magnetism in lattices of rings

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In this talk, we will show that ultracold atoms carrying Orbital Angular Momentum (OAM) in lattices of ring potentials are well suited candidates as quantum simulators of topological systems in the single-particle limit. In the Mott insulator limit, the system can realize a variety of spin-1/2 models, including the XYZ Heisenberg model with or without external field.

In the context of topology, we investigate the single-particle properties of a system formed by ultracold atoms loaded into the manifold of l=1 OAM states of an optical lattice with a diamond chain geometry [1,2]. Through a series of successive basis rotations, we show that the OAM degree of freedom induces phases in some tunneling amplitudes of the tight-binding model that are equivalent to a net π flux through the plaquettes and give rise to a topologically non-trivial band structure and protected edge states. In addition, we demonstrate that the system also exhibits Aharanov-Bohm caging. In two dimensional (2D) lattices, we also propose a realization of a 2D high order topological insulator [3]. We describe the system in terms of two decoupled lattice models, each of them displaying one-dimensional edge states and zero-dimensional corner states that are correlated with the topological properties of the bulk. Furthermore, we propose an alternative way to characterize the second-order topological corner states based on the computation of the Zak's phases of the bands of first-order edge states.

In the Mott insulator limit and at unit filling, a direct mapping between the OAM and spin-1/2 states can be performed [4]. We consider explicitly the dependence of the effective couplings on the geometry of the system and demonstrate that several models of interest related to a general XYZ Heisenberg model with external field can be obtained. Furthermore, we discuss how the relative strength of the effective couplings can be tuned and which phases can be explored by doing so in realistic setups.

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Coherent effects in atomtronic circuits.

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Atomtronics is an emerging field seeking to realize atomic circuits for quantum technology,exploiting ultra-cold atoms manipulated in micro-magnetic or laser-generated micro-optical cir-cuits. Indeed, several atomtronic circuits on small and medium size scale have been recentlyrealized experimentally. Important chapters in mesoscopic physics, like persistent currents inring shaped structures, transport through quantum dots and more complex terminals, quantumphase slips etc. could be explored with an enhanced flexibility and control. In this talk, I will give a brief overview of the field. In particular, In particular, I will be focusing on maybe the simplest instance of atomtronic circuit: ultracold-atoms in ringshaped potentials and pierced by an effective mag-netic flux and attached to leads

Kardar-Parisi-Zhang universality in 1D exciton-polariton systems

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Exciton-polaritons (EP) were shown to exhibit a Bose-Einstein condensation transition, which is genuinely out-of-equilibrium because of the driven-dissipative nature of this state [1]. Thus, its universal properties are likely to be different from the ones of an equilibrium condensate. Recently, it was suggested that the long-distance dynamics of the phase of the EP condensate follows the Kardar-Parisi-Zhang (KPZ) equation, a well-known model of classical statistical physics, and numerical hints of KPZ scalings were found in one dimension [2, 3]. However, the experimental accessibility of the KPZ regime was questioned. In this talk, I will present our results obtained by numerically solving the generalized Gross-Pitaevskii equation describing EP with realistic experimental parameters, which show that KPZ properties are indeed observable in current experimental set-ups [4]. Moreover, I will show that one-dimensional EP display fine features of KPZ universality class beyond the scaling exponents, concerning in particular the distribution of the phase fluctuations.

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Bell non-locality in many-body systems

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Elaborating on the seminal Einstein-Podolski-Rosen paper (1935), Bell introduced the concept of non-local correlations. The violation of Bell inequalities by the statistical correlations measured on quantum systems allows one to demonstrate a very non-classical, and puzzling, property of space-time. Very remarkably, such a demonstration is based on minimal assumptions. For instance, the quantum systems are treated as “black boxes”, with no specification about their physical nature, or even the validity of quantum mechanics. This feature is at the heart of the so-called “device-independent certification” of quantum devices – simulators, computers, etc.
Although originally introduced for a pair of correlated systems, Bell inequalities can be extended to multipartite systems. Multipartite Bell non-locality represents a very fundamental manifestation of quantum entanglement in many-body systems, which has remained largely unexplored, in spite of its crucial role in certification tasks. The mathematical complexity inherent to multipartite Bell inequalities, however, prevents from a generic and scalable approach to non-locality detection in many-body systems.
In a first part, I will present a strategy based on symmetric combinations of two-body correlators, leading to the discovery of permutationnally invariant Bell inequalities (PIBI) at ICFO a few years ago [Tura *et al*, Science 2015]. I will then show that the PIBI is violated close to the quantum critical point of the transverse-field Ising model – a physical consequence of the spin squeezing induced by quantum-critical correlations [Piga *et al*, arxiv. 2019]. Finally, I will discuss an alternative, generic data-driven approach to non-locality detection in many-body systems, formally equivalent to solving the inverse Ising problem [Frérot & Roscilde, in preparation].

Nonequilibrium thermodynamics of a driven dissipative quantum fluids of light

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Exciton-polaritons in semiconductor microcavities have been nowadays well established as a new class of quantum fluids, with defining phenomena such as Bose-Einstein condensation and Superfluidity [1]. Unlike ultra-cold atoms or liquid Helium, this unique class of fluid is characterized by the fact that the particles lifetime is in general too short to reach thermal equilibrium, and consequently, the fluctuations are nonthermal in origin, and stems from the particles joining and leaving the fluid.

This feature allows phenomena, that have no counterparts in thermal equilibrium quantum fluids, that will be the subject of this talk. We have shown for instance that heat from the fluid's solid-state environment (thermal phonons) can interact both weakly [2] and strongly [3] with the fluid of light, leading to unconventional energy transfers. We also found that in the superfluid state, the condensate interacts with an incoherent fluid in a way which is reminiscent of the "two-fluids" best describing superfluid Helium. But in our case, the two fluids are of different nature, and not at thermal equilibrium with each other, resulting in an unexpected behavior of the fluid speed of sound and critical velocity [4].

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D1 - Magnetism/oxide films 2: spintronics

ELECTRORESISTANCE IN EPITAXIAL FERROELECTRIC HfO_2-BASED THIN FILMS

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Discovery of ferroelectricity in HfO_2 films is a major breakthrough in material's science due to the well know integration of HfO_2 in current CMOS-compatible technologies and the possibilities that exploitation the ferroelectric polarization may offer to engineer new devices. However, the ferroelectric phase of HfO_2 is elusive an it appears to be a metastable phase competing with other polymorphs, thus challenging its growth and control. Opportunely, it has been lately reported the successful growth of epitaxial films of ferroelectric HfO_2-related compounds on single crystalline oxidic substrates [1,2], that may largely contribute to understanding the origin and nature of ferroelectricity in HfO_2. Here we will review our recent achievements, including the determination of the growth window for epitaxial growth of ferroelectric $Hf_{0.5}Zr_{0.5}O_2$ films and the role of some growth parameters (temperature, atmosphere and thickness) as well as the nature of the bottom electrodes and substrates on the stabilization of ferroelectric phase and its polarization-related properties.

…

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Spin-orbit torques in an ultrathin ferromagnetic metal layer between two oxides: quantum confinement and Rashba effect

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Since their experimental demonstration in the early 2010's, spin orbit torques (SOT) have generated significant interest in the magnetism and spin electronics communities. In heavy-metal (HM) / ferromagnetic metal (FM) / oxide (Ox) tri-layers, they allow the magnetization to be manipulated by means of a current injected into the layer plane, a writing principle that is the basis of a new generation of non-volatile memory, SOT-MRAM.
Nevertheless, although a great deal of work has been done to understand and optimize these SOTs, the physical origin of the two components of SOTs, the so-called “Field-like” (FL) and “Damping-like” (DL) torques, is still a source of debate: do they come mainly from the bulk of the HM through a Spin Hall Effect - type mechanism, or do they originate from the interfaces through a Rashba-type mechanism. Recent experimental studies have shown that the separation of these two contributions is difficult.
In order to study only one of these two mechanisms, the interfacial contribution, we studied SOTs in tri-layers without HM: Ox1/FM/Ox2. Despite the absence of HM and the almost symmetrical stack, we have highlighted evidenced their presence and shown that only the FL is present is such tri-layers. In addition, the unexpected behavior of this FL as a function of the thickness of the FM layer led us to propose a model based on the combination of a Rashba interfacial effect and a quantum confinement effect due to the very thin thickness of conductive material in these multilayers.

Probing antiferromagnets with currents

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The paradigm shift consisting of using the spin-dependent transport properties of antiferromagnets in electronics led to many exciting challenges.[1),2)]

In this talk, we will first discuss the nature of a spin current flowing through fluctuating antiferromagnets and distinguish between electronic and magnonic spin transport. The method used to inject the spin currents involved ferromagnetic resonance and spin pumping in ferromagnetic-spin-injector/(non-magnetic-spin- conductor)/antiferromagnetic-spin-sink multilayers. Three typical cases will be presented, magnonic spin flow in the insulating antiferromagnets NiO and NiFeOx, electronic spin flow in the metallic antiferromagnet IrMn, and electronic and magnonic parallel spin flows in IrMn when the latter is directly exchange coupled to the ferromagnetic-spin-injector. In this latter case, how it is possible to unravel the spin injection efficiency of the two types of spin flows will be demonstrated. We will also demonstrate how linear spin fluctuations enhance spin injection in spin-sinks and show why this is pertinent for studies of critical phenomenon like magnetic phase transitions in ultra-thin films. To show the far-reaching practical relevance of the method, extension to various phase transitions will be presented.[3)-6)]

In search for spin fluctuations in several antiferromagnetic spin-sinks, we will also discuss how we found experimental evidence of self-induced spin-charge conversion in the spin-injector, corroborating the results of first-principle calculations.[7),8)]

Beyond spin currents, we will finally present a stimulating example of how antiferromagnets and superconductors may envision a common future by showing how to infer essential information about domain walls using Cooper pairs through antiferromagnets.[9),10)]

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Magneto-ionic effects in nanoporous iron oxides

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Voltage control of the magnetic properties of oxide thin films is highly appealing to enhance energy efficiency in miniaturized spintronic and magnetoelectric devices [1]. Iron oxide system is of particular interest because iron is cheap and environmentally-friendly and there are multiple iron oxide phases that are stable at room temperature which all have distinct magnetic properties [2,3]. Herein, magnetoelectric effects in electrolyte-gated nanoporous iron oxide (FeO_x) films are investigated. Highly porous films were prepared by the evaporation-induced self-assembly of sol-gel precursors with a sacrificial block copolymer template. For comparison, films with less porosity but analogous crystallographic structure were also prepared using an identical procedure without the polymer template. The magnetoelectric properties of the films were investigated by recording magnetization *vs.* magnetic field loops as a function of applied voltage. An electrochemical cell is used to apply electric fields *in situ*, i.e., while the magnetic properties of the films are being measured. The templated (highly porous) films showed a very large magnetoelectric response with a maximum increase in magnetic moment at saturation by a factor of 13 and a noticeable two-fold increase of coercivity after applying –50 V [4]. The non-templated films also exhibited a pronounced increase of magnetic moment at saturation by a factor of 4, although the coercivity remained unaffected over the same voltage range. Magnetoelectric effects in these latter films were found to be fully reversible in the voltage window ±10 V. The observed changes in magnetic properties are concluded to be magneto-ionically driven, as evidenced from Raman and X-ray photoelectron spectroscopy experiments.

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Oxidation dependence of the Dzyaloshinskii-Moriya interaction in Pt/Co/MO_x trilayers (M = Al or Gd)

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We have studied the interfacial Dzyaloshinskii-Moriya interaction (DMI) in Pt/Co/MO_x (M = Al, Gd) trilayers in which the degree of oxidation of the top Co interface is varied [1]. To access reliable values of the DMI strength, we have used a method based on the measurement of the saturation velocity of field driven chiral Néel domain walls. We show that the effective DMI strength in the Pt/Co/MO_x trilayers varies with the oxidation degree of the Co/MO_x interface. This strongly suggests that the Co/MO_x interface gives a distinct contribution to the total DMI, adding to that of the Pt/Co interface. The DMI presents a maximum for the oxygen coverage maximizing also the interface magnetic anisotropy energy K_s. This calls for common microscopic origins for the contributions of the Co/MO_x interface to DMI and K_s.

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Magnetoelectric effects in mesoporous alloys: towards enhanced energy efficiency in magnetically-actuated devices

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Magnetic storage systems and magnetically actuated devices in general are ultimately controlled by magnetic fields generated using electric currents. This involves significant power dissipation by Joule heating effect. To optimize energy efficiency, manipulation of magnetic information with lower magnetic fields (i.e., lower electric currents) is desirable. This can be accomplished by reducing the coercivity of the actuated material by, for example, an externally applied DC voltage (i.e., electric field). In recent years, we have observed a drastic reduction of coercivity at room temperature in a variety of relatively thick (>500 nm), nanoporous films, including Cu-Ni, Cu-Fe or Co-Pt alloys. These films (which can be also patterned using lithographic procedures) are typically prepared by micelle-assisted electrodeposition. The voltage is applied across an electrical double layer using a non-oxidative liquid electrolyte (propylene carbonate with Na^+ solvated species). Magnetoelectric effects arise from modification of the 3d electronic band structure of these alloys, together with oxygen migration (in case oxygen is made available in the system, i.e., by magneto-ionics). The large surface-area-to-volume ratio and the ultra-narrow pore walls of these systems allow the whole films, and not only the topmost surface, to effectively contribute to the observed magnetoelectric effects. This allows for the observation of voltage-driven changes in coercivity that are much larger than those observed in some previous studies on ultra-thin (1-2 nm) magnetic films. The voltage-induced decrease of coercivity could be used as an alternative to thermally-assisted magnetic writing in magnetic recording applications, since the latter is less energetically effective. The results from this work also serve to expand the already wide range of applications of nanoporous materials (hitherto in areas like energy storage or catalysis) and it opens new paradigms in the fields of spintronics, computation and magnetic actuation in general.

D2 - 2D Materials

In situ investigation of graphene growth on liquid copper

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The aim of the LMCat (liquid metal catalysis) EU Horizon 2020 project is to deliver an instrumentation and methodology allowing to study in situ and in operando the growth of 2D materials (2DMs) on liquid metal surfaces.

The current approach to graphene (Gr) synthesis generally relies on CVD growth on solid substrates, mainly copper. Despite recent progress and fine-tuning of growth procedures there are significant obstacles in transferring the current knowledge towards mass production of good quality sheets over large-scales. The main showstoppers are slow procedures of 2DMs separation from solids, their environmental unfriendliness, and low quality of produced layers. All these factors significantly impact process costs, speed, and waste production.

In this contribution we will present the first experimental results of graphene growth on liquid copper in a newly developed CVD reactor, dedicated to the study of chemical reactions on LMCats. By combining in situ synchrotron X-ray diffraction and optical microscopy, supported by ex situ Raman spectroscopy, we are capable to resolve in real-time the growth dynamics and atomic structure of graphene during its growth on liquid copper. Contradictory to solid, this later is an atomically smooth, isotropic and mobile medium, which allows to produce graphene crystals of extremely high-quality and large sizes limited only by the liquid bath surface. A myriad of interesting growth scenarios was observed which allowed to fine-tune the fabrication procedures and to identify key factors impacting the growth of individual flakes, their self-assembly and further association into a single layer with a coherent atomic structure.

The obtained results are indispensable for establishing the methodology for the continuous production of graphene sheets on LMCats and pave a new way for the future cost-effective and large-scale fabrication of 2DMs.

Atomic defects in 2D materials studied by transmission electron microscopy

Hanako Okuno

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Structural defects are considered as a parameter-tuning knob for tailoring physical properties of 2D materials. The ability to engineer atomic defects at nanometer scale opens up unique opportunities to alter and enhance electrical, optical, mechanical and magnetic properties. Despite the growing interest in 2D materials, growing defect-free 2D materials on desired substrates remains a challenge. Identification and characterization of these inevitable intrinsic growth defects are thus an essential process. Further exploitation of possible defect modification and manipulation might shed light on potential utilization of defect structures in device processing. Aberration Corrected Transmission Electron Microscopy (AC-TEM) is one of the most suitable techniques to study the atomic structure of 2D materials, which enables to visualize atomic defects and simultaneously to form new defects by electron irradiation. In this work, we study the atomic defects in various synthesized 2D layers, as grown and after processing such as annealing and irradiation, using multiple advanced AC-TEM techniques to explore the possibilities of defect engineering and materials design by combining their intrinsic and extrinsic defects.

Perpendicular magnetic anisotropy, unconventional spin texture and extraordinary gradual spin reorientation transition of cobalt films in contact with graphene

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Owing to its peculiar electronic band structure, high carrier mobility and long spin diffusion length, graphene is a promising two-dimensional material for microelectronics and spintronics. Graphene also shows interesting magnetic properties when in contact with a ferromagnetic metal (FM). For instance, graphene carries a net magnetic moment when deposited on Fe/Ni(111), and a significant spin splitting can be induced in graphene due to proximity with a heavy element.

While these results illustrate potential advantages of integrating graphene within a magnetic stack, the influence of graphene on the magnetic properties of a FM is still largely unexplored. In particular, non-magnetic overlayers generally affect the magnetic anisotropy energy (MAE) of thin layers, where interfaces play an important role. We can then wonder how an interface with graphene would influence the MAE of a thin FM film.

Using spin-polarized low-energy electron microscopy, we study how a graphene overlayer affects the magnetic properties of atomically flat, nm-thick Co films grown on Ir(111). In this contribution, we report several astonishing magnetic properties of graphene-covered Co films:
1) Perpendicular magnetic anisotropy is favored over an unusually large thickness range,
2) Vectorial magnetic imaging reveals an extraordinarily gradual thickness-dependent spin reorientation transition (SRT),
3) During the SRT, cobalt films are characterized by an unconventional spin texture,
4) Spectroscopy measurements indicate that incident spin-polarized electrons do not suffer substantial spin-dependent collisions a few electron-Volts above the vacuum level.

These properties strikingly differ from those of pristine cobalt films and could open new prospects in surface magnetism and spintronics.

D3 - Quantum circuits, quantum thermodynamics and quantum information

The energetic cost of quantum control

Alexia Auffeves
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Quantum Thermodynamics is an emerging and interdisciplinary field, that is currently building its own concepts with material taken from quantum information, quantum open systems, stochastic and information thermodynamics. It addresses a vast range of questions, whether fundamental or applied, e.g. What is the nature of time arrow at the quantum scale? How does it impact the efficiency of quantum engines? Are quantum coherence and entanglement new energetic resources? What is the energetic bill to run a quantum protocol?…

In this talk I will focus on a recent proposal of Maxwell's demon engine where work is not extracted from thermal fluctuations, but quantum fluctuations induced by quantum measurement only [1]. This "measurement driven engine" has unlocked a new research line and offers a striking illustration of the thermodynamic footprint of measurement in the quantum regime, which acts as the ultimate source of randomness, irreversibility, and energy [2]. I will then switch to the autonomous version of this engine, where work is extracted from an engineered bath acting as a source of energy and coherence [3]. This last proposal sheds new light on how coherence impacts work extraction in the quantum regime. I will finally focus on the opposite side of quantum thermodynamics as a tool to assess the energetic cost of running quantum protocols against quantum noise [4].

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Quantum Computing at IFAE

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Institut de Física d'Altes Energies
& Barcelona Supercomputing Center

Quantum Computing has moved in recent years from purely quantum algorithms, highly challenging to implement, to hybrid ones combining classical techniques which may be run on small-sized devices prone to errors in the near term. In this presentation, I am going to introduce the newly created Quantum Computing Technology Group at IFAE. The focus of the group is to develop a coherent superconducting quantum annealer to perform optimization tasks, as well as quantum simulation operations. In addition, some interests will be placed on the bridge towards high energy physics.

Many-body physics with superconducting quantum circuits

Nicolas Roch
Institut NEEL, CNRS, & Université Grenoble Alpes

During this presentation, I will first review the various building blocks and concepts used in the frame of superconducting quantum circuits: superconducting resonators, superconducting qubits and microwave photons. I will then explain how to arrange them to build circuits, which exhibit quantum many-body behaviors similar to what is usually observed in condensed matter physics. I will finally illustrate this point using recent experimental results.

Advanced magnetocaloric materials for low-temperatur refrigeration

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Low-temperature refrigeration is crucial to emergent quantum information technologies as well as to many other scientific applications stretching from space telescopes to medicine. This fuels a growing interest in alternative refrigeration methods capable to compete with standard liquid-helium cryostats. One of such cooling technologies is the adiabatic demagnetization refrigeration (ADR) based on the magnetocaloric effect. The existing ADR technologies for the sub-Kelvin range utilize dilute paramagnetic salts of Cr and Fe magnetic ions, which proved to have limited efficiency at higher temperatures. It has been recently demonstrated that geometrically frustrated magnets with a residual ground state degeneracy exhibit a very strong magnetocaloric effect [1,2,3]. I shall survey theoretical background of the magnetocaloric effect in frustrated and low-dimensional magnets. In addition, new results of the IRIG–Institut Néel collaboration on the promising magnetocaloric material $Yb_3Ga_5O_{12}$ will be presented. I shall discuss general directions of the search of newpr ospective refrigerant materials by exploring collective effects in systems of interacting magnetic moments as opposed to noninteracting moments in paramagnetic salts.

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Dynamically induced heat rectification in quantum systems

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Heat rectifiers are systems that conduct heat asymmetrically for forward and reversed temperature gradients. Here, I will present present the study of heat rectification in linear quantum systems and demonstrate that asymmetric heat currents can be induced in a linear system only if it is dynamically driven. The rectification can be further enhanced, even achieving maximal performance, by detuning the oscillators of the driven network. I will explain the consequences such a scheme can have in future applications.

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Poster Session

Long range coupling of magnetic bilayers by coherent phonons

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SPINTEC, Grenoble

We demonstrate that the spin waves can be strongly coupled to coherent shear waves that have very long characteristic decay length and propagate ballistically over millimetric distances. In our spin valve structure, which consists of two insulating magnetic layers (YIG) deposited on both sides of a dielectric GGG substrate, the standing acoustic waves couple to the magnetization oscillations in both layers. The coupling signifies a change of sign between the acoustic modes with even or odd indices, which results in a contrast between two tones separated by half a wavelength. We measure the contrast at different polar angles via inverse spin Hall effect using a thin Pt wire deposited on one side of the YIG layer. In our sample the two YIG layers resonate at slightly different frequencies. The change in the polar angle allows to detune their resonances and make them cross, which leads to a peak of the contrast at the crossing point. We show that the observed behavior is in agreement with theoretical prediction. This long range coherent coupling by phononic angular momentum currents adds new functionalities to insulator spintronic circuits and devices.

Integration of Tb/Co Multilayers within Ultrafast Optically Switchable p-MTJ

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Rare earth/transition metal (RE/TM) systems have been used to achieve perpendicular anisotropy in RE/TM multilayers. The discovery of all-optical switching of the magnetization, achieved on ultrafast timescales using femtosecond laser pulses have generated a renewed interest in these type of systems for data-recording applications. In particular, the ultrafast speed of the switching process permits a significant improvement in the writing speeds associated with magnetic memory devices.
This work reports the development of perpendicular magnetic tunnel junction, incorporating a multilayered stack of Tb/Co that can be all-optical addressed via helicity-independent single-shot switching of the magnetization. Toggling of the magnetization in the Tb/Co multilayered stack was observed using both 60 femtosecond- and 5 picosecond-long laser pulses with fluences below 5mJ/cm². As illustrated in Fig. 1, these results could be achieved for Co-rich compositions of the multilayer, either alone or embedded in a tunnel junction stack coupled to a CoFeB electrode on an MgO barrier. This result is maintained even after annealing at 250°C. After annealing, a TMR signal of 30% and RxA value of 19 Ωμm² was obtained.
The stability of the multilayer degrades for higher annealing temperatures. This is due to a loss of the interface sharpness that could be compensated by the increase of the number of bilayer repetitions. The annealing stability of the multilayer was improved using a Ta insertion layer, at the cost of reducing the strength of the perpendicular anisotropy and magnetic coercivity. These results open the way to the development of hybrid spintronic photonic systems with unique features of THz MTJ switching speeds and fJ switching energies
The authors acknowledge the funding support from project SPICE (EU ITC 2020 grant agreement No. 713481)

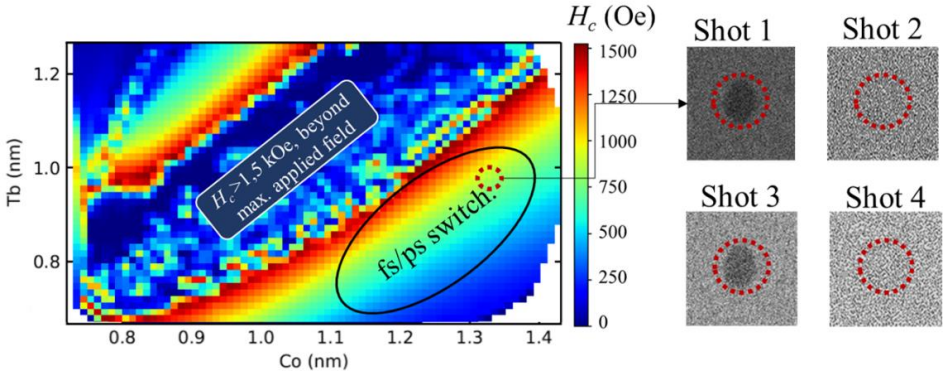

Fig. 1 Left: Coercive field mapping of half-MTJ structure for different values of Co and Tb thickness. Right: Magneto-optical switching experiments performed for a FeCoB/Ta/[Tb(1 nm)/Co(1.3 nm)] half-MTJ stack annealed at 250°C after 4 shots of the 5 ps-laser pulse with fluence ~ 4.7 mJ/cm².

Single Molecular Magnet, a fascinating platform for quantum experiments

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The realization of a universal quantum computer is one of the major scientific objectives of the 21st century, as its promises are revolutionary: inviolable cryptography, higher computing power, simulation processes inaccessible to conventional technologies ... Its principle is based on qubit, a two-level quantum system, a quantum analogue of the classical bit. Today, the challenge is to increase the number of qubits in interaction to achieve more complex and more efficient quantum information protocols. In this context, molecular magnets of nanometric size are of major interest. The information is carried by the direction of magnetization which is multiple, unlike conventional magnets which have only two. They thus make it possible to have d-states quantum devices or qudits. These multi-level devices could the processes involved in the manipulation of quantum spin more efficient. The use of these would also simplify some computational tasks, and thus the circuits required to realize a quantum computer

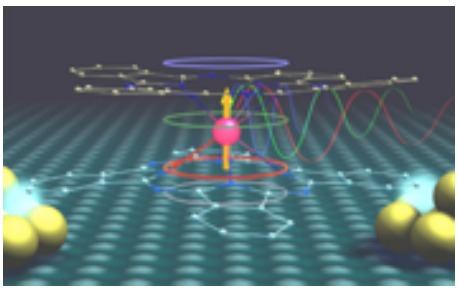

Fig. : Artist view of a a single magnet molecular transistor. The heart of the circuit is the terbium-based molecular magnet (pink): two planar organic molecules protecting the Terbium ion. The magnet is connected to two metal electrodes (gold atoms) deposited on a substrate. The reading of the four spin states of the nucleus (represented in the magnification in the form of colored rings) is performed by an means of electric current. The exploration of the quantum properties of this is obtained by the application of microwave electric field pulse (blue, green and red)

In this context, it is possible to fully control a multilevel system based on a single molecular magnet. Proving that it is possible to read-out and manipulate the four-level spin of the terbium nucleus of a molecule was a first step to show the long decoherence time of a single nuclear spin which is by nature strongly isolated from its environment[1].

Among those properties, superposition of states and phase interference are two fundamental mechanisms from which quantum computing can benefit. We explored these properties by applying 3 interference protocols involving the phases of the four nuclear spin states[2]. A first measurement makes it possible to know the coherence time of the coherent superposition of a quantum system. Applied to a coherent superposition of three nuclear spin states, this protocol can be generalized to any given qudit. The second protocol makes it possible to directly measure the final phase of a quantum state on which different quantum gates where applied. It is an essential tool for the development of quantum algorithms. Finally, in a physical system that evolves adiabatically and cyclically, one can highlight, a phase that depends on the entire evolution during a cycle.

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2. Generalized Ramsey Interferometry Explored with a single nuclear spin Qudit **.** C. Godfrin, R.Ballou, E. Bonet, M. Ruben, S. Klyatskaya, W. Wernsdorfer and F. Balestro. *Npj Quantum Information* **4**, 53 (2018)

hBN encapsulated liquid-gated graphene field-effect transistors : toward sensitive and stable sensors in liquid medium.

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Great efforts are currently devoted to the development of liquid-gated graphene field-effect transistors (g-FET) as sensor for biomedical applications and particularly, neural interfacing. Indeed, due to its high carrier mobility, graphene based sensor devices show, with PEDOT-PSS, the highest sensitivity ever reported. Transferred on a proper substrate, its flexibility is also a clear advantage for implantable technology by reducing the rejection from the biological tissue. However, at this stage, g-FETs did not show their full potential. Actually, since the graphene channel is in direct contact with the liquid medium, the carrier mobility stays below its theoretical value and the devices are subjects to stability issues. Moreover, the presence of electrical 1/f noise, whom origin is not well understood, is also a limitation for the device miniaturization. In this study, we suggest that graphene encapsulation in hexagonal Boron Nitride (hBN) could be a solution to overcome those problems. Besides boosting the carrier mobility, we expect that the presence of a «spacer » between the graphene monolayer and the surrounding impurities and charge traps would decrease the 1/f noise and protect the channel from the degradation in the liquid. In this poster, series of encapsulated and non-encapsulated g-FETs, fabricated with CVD graphene grown on Copper foil and transferred on doped Si/SiO_2 substrates is presented. The graphene quality is assessed by Raman Spectroscopy. Mobility (extracted by Hall Effect) and noise measurements in the top-gate and back-gate configuration without or in the presence of liquid is reported and discussed.

Ion-gel gated single layer MoS2 transistors as switch for multiplexing applications

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Thanks to its low dimensionality and large intrinsic band gap, MoS2 is an interesting semiconductor for future flexible and wearable electronics. In the optic of high density mapping and stimulation of brain activity, our team is currently working on the elaboration of MoS2 flexible switches to perform time division based multiplexing of liquid-gated graphene field-effect transistors (g-FET) matrix. In this framework, the use of solid-polyelectrolyte as gate material to enable both flexibility and low powering is explored. Indeed, thanks to the high capacitive coupling between the ionic gel and the 2D layer, the gate voltage required to open the MoS2 channel can be decreased by a factor 5 to 10 compared to standard dielectrics.

In this study, we report on the growth and characterization of ion-gel gated MoS2 field-effect transistors. First, the growth of MoS2 closed layers in a home-made reactor is described. Two different substrates are used for the deposition: standard Si/SiO2 and Na-containing silicate glass. The resulting monolayers, characterized by Scanning Electron Microscopy, Raman Spectroscopy and X-Ray Photoemission Spectroscopy are compared.

In order to be used as switches to address g-FET matrix, MoS2 devices should fulfil several criteria ; high ON/OFF ratio and switching speed and, be able to carry hundreds of μA current without addition of noise in the ON state. For this reason, we decided to process our layers in an interdigitated configuration. The performances and limitations of the transistors (ON-OFF ratio, threshold voltage, switching speed, noise…) will be discussed.

On the Role of Interfaces on Spin Transport in Magnetic Insulator/Normal Metal Heterostructures

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Exploitation of pure spin currents has emerged as a new tool in spintronics, with promises of more efficient devices in data storage and computing. A pure spin current can be generated in a non-magnetic metallic (NM) layer by a charge current (spin Hall effect, SHE). The reciprocal effect, the inverse Spin Hall effect (ISHE), converts a pure spin current in to a charge current. Many devices using SHE and ISHE, involve spin transport across interfaces between non-magnetic metallic layers and magnetic materials; quiet commonly, magnetic insulators. The structural, compositional and electronic differences between these materials and their integration to form an interface, challenge the control and understanding of the spin transport across it, which is known to be sensitive to subnanometric interface features. We will illustrate some of these difficulties and show how spin currents can be used as a probe for surface magnetism.

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Correlated electronic systems as transparent conductors

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Transparent metallic oxides are pivotal materials in information technology, photovoltaics, or even in architecture. They display the rare combination of metallicity and transparency in the visible range because of weak interband photon absorption and weak screening of free carriers to impinging light. However, the workhorse of current technology, indium tin oxide (ITO), is facing severe limitations and alternative approaches are needed. AMO_3 perovskites, M being a nd^1 transition metal, and A an alkaline earth, have a genuine metallic character and, in contrast to conventional metals, the electron–electron correlations within the nd^1 band enhance the carriers effective mass (m) and bring the transparency window limit (marked by the plasma frequency, ω_p*) down to the infrared. We will show that epitaxial strain and carrier concentration allow fine tuning of optical properties (ω_p*) of $SrVO_3$ films by modulating m* due to strain-induced selective symmetry breaking of 3d-t_{2g}(xy, yz, xz) orbitals. Interestingly, the DC electrical properties can be varied by a large extent depending on growth conditions whereas the optical transparency window in the visible is basically preserved [1]. These observations suggest that the harsh conditions required to grow optimal $SrVO_3$ films may not be a bottleneck for their future application.*

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Wafer-scale growth of layered III-VI materials by MOCVD

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III-VI materials are an emerging class of layered semiconductors with very interesting electrical and optical properties. High performance field effect transistors[1], photodetectors[2], light emitters[3] and second harmonic generators[4] has already been widely demonstrate using these materials. Nevertheless, as for all 2D materials, their integration in real world applications will only be possible if a large scale/high yield fabrication method can be achieved using the standard tools present in a foundry.

In this work we will present a fast and uniform MOCVD growth process of highly oriented micronic domains of GaSe, InSe and their van der Waals heterostructures on large diameter Si(001) and Si(111) wafers. The growth mechanisms at the atomic scale will be discussed from AFM images, high resolution STEM, X-ray diffraction measurements and density functional theory calculations.

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Extracting topology through optical diffraction: a study of the Integer Quantum Hall Effect in two, three and four dimensions

Crystal electrons in uniform magnetic fields display a series of striking properties, like a fractal spectrum [1] and a quantized conductance [2]. For a rational (adimensional) magnetic flux piercing the lattice, $\phi = p/q$ with co-prime integers p and q, the system has an energy spectrum made by q smooth bands. Each of these bands is characterized by an integer topological invariant called the Chern number and, whenever the Fermi energy is set in a gap, the (adimensional) transverse conductance is given by the sum of the Chern numbers of the occupied bands. This phenomenon, the Integer Quantum Hall Effect (IQHE), firstly observed in a two dimensional (2D) system, takes place also in three dimensional (3D) [3] and four dimensional (4D) [4] systems. As first discussed by Wannier, the geometrical structure of a crystalline potential in a magnetic field reflects on the "statistical weight of the spectrum" (or integrated density of states), which is simply the fraction of occupied bands. This may be conveniently displayed in terms of so-called *Wannier diagrams*, which render evident how the density of states grows linearly with the magnetic flux [5]. The subsequent theory of 2D IQHE developed by Thouless and coworkers [6] on the Hofstadter model, and by Streda [7], proved that the linear coefficient which links the density of states and the magnetic flux is proportional to the Hall conductivity (Streda-Widom formula). In particular, these studies highlighted that the complete topological information about the system is fully encoded in its Wannier diagram. This applies also to the generalizations of the Hofstadter model to three [3] and four [4] dimensions. Recently, the topology of a one-dimensional quasicrystal was probed through a diffraction experiment [8]. This experiment required direct access to the complex phase of the diffracted wave. The latter was ingeniously extracted through an interferometric experiment. Here, instead, we probe the topology of three different crystalline potentials, in two, three and four dimensions, by measuring the intensity (i.e., the squared amplitude) of the diffracted fields: for each potential, we measure the diffraction figure at different values of the grating's period. This allows us to recover the Wannier diagram of the corresponding crystalline potential and to extract the Chern numbers of the different spectral gaps with the help of the Streda-Widom formula.

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Angular Momentum Fractionalization for Attracting Bosons in Ring-Shaped Potentials

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Quantum mechanics is characterised by quantum coherence and entanglement. After having discovered how these fundamental concepts govern the physical reality, scientists have been devoting intense efforts to harness them to shape future science and technology. This is a highly nontrivial task because most often quantum coherence and entanglement are difficult to access. Here, we present a quantum many-body system in which quantum coherence and entanglement explicitly demonstrate the quantum advantage of quantum technology over the classical one. Our physical system is made of strongly correlated, attracting neutral bosons flowing in a ring-shaped potential of mesoscopic size. Quantum analogues of bright solitons are formed in the system by the attractive interactions, and, as a genuine quantum-many-body feature, we demonstrate that an angular momentum fractionalization occurs. As a consequence, the matter-wave current in our system is able to react to very small changes of rotation or other artificial gauge fields. We discuss how our results put the basis to devise rotation sensors and gyroscopes with enhanced sensitivity.

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Tunable bipolar resistive switching in TiN/$LaMnO_{3+\delta}$/Pt heterostructures

As the need of increasing data storage arises, new candidates for non-volatile memories are required. Valence change memories (VCM) are one of the promising ones given their recent performance demonstrations in terms of switching time, switching energy and retention[1]. Resistive switching (RS) in VCMs occurs due to the drift of oxygen vacancies together with the concomitant redox reaction at the nanoscale.

A TiN/$LaMnO_{3+\delta}$ (LMO)/Pt heterostructrure was chosen to build our VCM nanoionic devices, as LMO is able to accommodate a flexible oxygen stoichiometry by varying the Mn^{3+}/Mn^{4+} ratio. Polycrystalline thin films were prepared on platinized silicon [2] with TiN electrodes sputtered on top, obtaining devices in "top-bottom" configuration. The TiN/LMO/Pt devices can be operated both in a counter clock wise (CCW) or in a clockwise (CW) regime, being the change in switching direction highly dependent on the induced current asymmetry. While the CCW regime shows highly reproducible RS with HRS/LRS ratios between 2 and 10 and endurances of up to 100 cycles, the CW regime presents endurances of only a few cycles, and HRS/LRS ratios which are comparable or smaller to those of the more stable and reproducible CCW regime.

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Investigating spin Hall angle and transparency in Py/Ta based heterostructure using Spin-torque FMR

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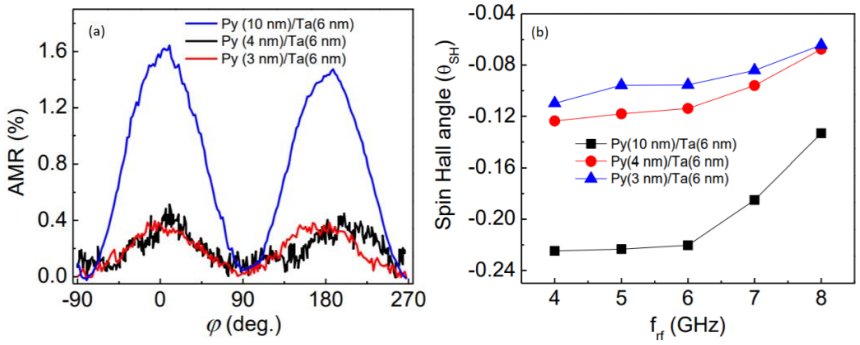
Abstract: The magnetization dynamics in the Py/Ta heterostructure is studies using spin Hall effect of Ta via spin torque ferromagnetic resonance. Gilbert damping constant was evaluated and found to increase as the thickness of ferromagnetic layer decrease. Our experimental results on thinner Py films shows lower anisotropic magnetoresistance and has low signal-to-noise ratio compared to thicker Py films. We calculated transparency which plays an important role on the magnitude of spin Hall angle. We found a direct relation with transparency at the Py/Ta interface and the magnitude of spin Hall angle showing high spin Hall angle for thicker Py films on Ta.



(a) AMR of the device as a function of in-plane angle φ (angle between I_{rf} and H_{ext}). (b) Dependence of θ_{SH} as a function of f_{rf} for different Py thickness.

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Correlated Quantum Tunnelling of Monopoles in Spin Ice

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The spin ice materials $Ho_2Ti_2O_7$ and $Dy_2Ti_2O_7$ are by now perhaps the best-studied classical frustrated magnets. A crucial step towards the understanding of their low temperature behaviour – both regarding their unusual dynamical properties and the possibility of observing their quantum coherent time evolution – is a quantitative understanding of the spin-flip processes which underpin the hopping of magnetic monopoles. We attack this problem in the framework of a quantum treatment of a single-ion subject to the crystal, exchange and dipolar fields from neighbouring ions. By studying the fundamental quantum mechanical mechanisms, we discover a bimodal distribution of hopping rates which depends on the local spin configuration, in broad agreement with rates extracted from experiment. Applying the same analysis to $Pr_2Sn_2O_7$ and $Pr_2Zr_2O_7$, we find an even more pronounced separation of timescales signalling the likelihood of coherent many-body dynamics.

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Randomized measurements: A toolbox for probing quantum simulators and quantum computers

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Experiment: T. Brydges[1,2], M. Joshi[1,2], C. Maier[1,2], P. Jurcevic[1,2], B. Lanyon[1,2], R. Blatt[1,2], C. Roos(1,2)

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Abstract

Randomized measurements have emerged as a new tool to probe the properties of quantum simulators and quantum computers beyond standard observables. In the poster I summarize our recent results including randomized measurement protocols to measure entanglement [1], out-of-time-ordered correlations [2], many-body topological invariants [3], and quantum state fidelities [4]. I will also show some experimental results [4,5,6] obtained in collaboration with the group of Rainer Blatt (IQOQI Innsbruck).

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A non-equilibrium system as a demon

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Maxwell demons are creatures that are imagined to be able to reduce the entropy of a system without performing any work on it. Conventionally, such a Maxwell demon's intricate action consists in measuring individual particles and subsequently performing feedback. Here we show that much simpler setups can still act as demons: we demonstrate that it is sufficient to exploit a non-equilibrium distribution to seemingly break the second law of thermodynamics. We propose both an electronic and an optical implementation of this phenomenon, realizable with current technology.

R. Sánchez, J. Splettstoesser, R.S. Whitney, to appear in Phys. Rev. Lett. (2019) — arXiv:1811.02453

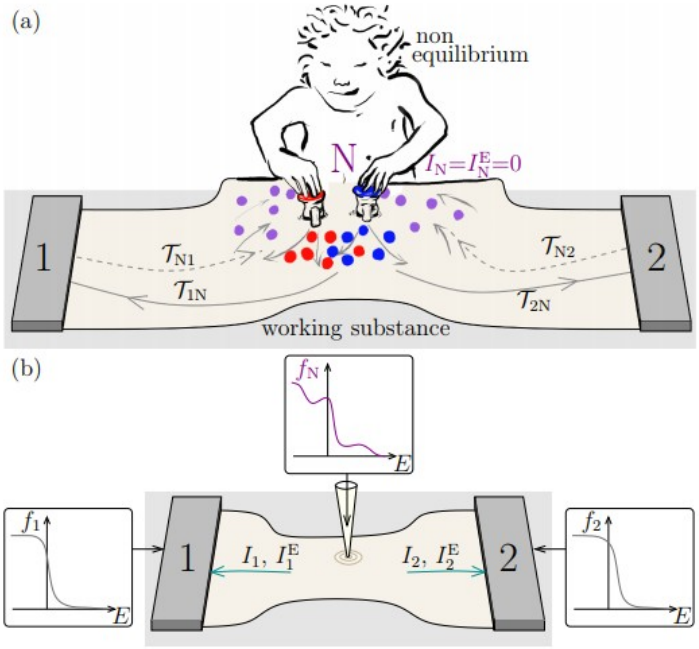

Figure 1. (a) The N-demon supplies a non-equilibrium distribution to the working substance (containing equilibrium reservoirs 1 and 2), without supplying heat or work. The non-equilibrium distribution could be a non-thermalized mixture of different equilibrium distributions. Transmission probabilities, $\mathcal{T}_{ij}$, of the scattering region (beige) involving terminal N are indicated and accompanied by grey arrows. (b) A physical implementation in which the non-equilibrium distribution f_N is injected locally into the working substance.

Why magnetic cooling is "hot:" theoretical and experimental perspectives

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Adiabatic demagnetization refrigeration based on the magnetocaloric effect is one of the simplest and environment-friendly cooling techniques. It is routinely used for low temperatures, typically in the sub-Kelvin regime, employing paramagnetic salts. Recent advances in the field of frustrated magnetism suggest them as very effective refrigerant materials. I shall survey theoretical background of the magnetocaloric effect in frustrated magnets and present experimental results on the garnet Yb3Ga5O12, which is a new very promising magnetocaloric material for low-temperature refrigeration.