Réunion thématique du GDR MEETICC:

De la matière quantique aux matériaux fonctionnels / From quantum matter to functional materials

Paris, January 24-25, 2023

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24-24 janv. 2023

Matériaux solides pour le stockage et/ou la conversion de l'énergie

Batteries and Solid State Physics: An Inseparable Link

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(Professor at College de France)

Batteries, as one of the most versatile energy storage technologies, play a central role in the ongoing transition from fossil fuels to renewable energy. Therefore, the enhancement of the battery performance, reliability, longevity and sustainability becomes a crucial challenge for the years to come. To address these various aspects, disruptive approaches enlisting either new materials, new reactivity concepts or new diagnostic tools to monitor intertwined complex physical/chemical processes within the battery under real working conditions are needed. This presentation will first recall that physicists were the first to study the type of materials (oxides or chalcogenides) used in Li-ion batteries. Afterwards the interlink between both physics and chemistry will be describe trough specific examples dealing with either the new concept of anionic redox or the use of fiber optics sensors to monitor the state of health of batteries to name only a few. .

Matériaux pour l'électronique du futur

Correlated quantum materials for microelectronic applications

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Mott insulators are correlated quantum materials that should be metallic according to conventional band theory, but are insulating due to strong on site electron-electron repulsions. In the last decades, Mott insulators have been the subject of intense research. Indeed, electron doping or pressure can cause insulator to metal transitions in these materials and lead to remarkable properties. Nevertheless, the difficulty to control external parameters such as pressure or doping in microelectronic devices makes the use of Mott insulators in microelectronic applications still scarce. Recent works have therefore focused on a new way to destabilize the Mott insulator state and induce an insulator to metal transition by using electric field. This transition, called "Electric Mott Transition", as for main signature a resistive switching controllable by electric pulses, which is very promising in terms of microelectronic applications. It could therefore open the door to new electronics based on Mott insulators, namely Mottronics.

This presentation will first review the electric Mott transition and the new functionalities enabled by this property. In a second time, it will present some examples of Mottronic devices in particular for data storage or artificial intelligence applications.

Transverse barrier formation by electrical triggering of a metal-to-insulator transition in LSMO and magnetoresistance effects

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Combing resistive switching and spintronic functionalities in a single device is an exciting opportunity to bring together the advantages of charge- and spin-based electronics, enriching the design space for practical applications, and to further the basic understanding of interactions between electrical and magnetic properties of materials. Here we explored magnetotransport in ferromagnetic oxide $(La, Sr)MnO_3$ $(LSMO)$ during electrical triggering of the intrinsic metal-insulator transition (MIT), which produces volatile resistive switching. This switching occurs in a characteristic spatial pattern, the formation of a paramagnetic insulating barrier perpendicular to the current flow, in contrast to the conventional filamentary percolation parallel to the current. At the threshold voltage of the MIT triggering, we observed strong anomalies including large magnitude increase and flipping of the sign of anisotropic and colossal magnetoresistances. We attributed those anomalies to the coupling between the voltage induced paramagnetic insulating barrier formation and intrinsic magnetoresistance. Additionally, we will discuss the behaviours of a newly designed hybrid optoelectronic heterostructure that uses photocarrier injection from cadmium sulfide (CdS) to an $LSMO$ layer to change its electrical conductivity. Although $LSMO$ is known to have no significant optical response, our ultrathin film CdS/LSMO heterostructures show enhanced conductivity with ≈ 37 % resistance drop at transition temperature under light stimuli. This enhanced conductivity in response to light resembles the effect of applying a 9 T magnetic field in pure $LSMO$. Furthermore, optical and magnetic responses in our heterostructures are found surprisingly to be decoupled when both stimuli are applied. Our work demonstrates a novel approach to manipulate magnetic properties by electrically driving the material into the out-of-equilibrium resistive switching state.

This work was supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES), Materials Sciences and Engineering Division under Award # DE-FG02- 87ER-45332.

P. Salev, L. Fratino, D. Sasaki, R. Berkoun, J. Del Valle, Y. Kalcheim, I. K. Schuller, **Transverse barrier formation by electrical triggering of a metal-to-insulator**

transition. Nature communications, 12(1), 2021 https://www.nature.com/articles/s41467-021-25802-1

H. Navarro, L. Fratino, S. Bag, T. D. Wang , E. Qiu, V. Rouco, I. Tenreiro, F. Torres, A. Rivera-Calzada, J. Santamaria, M. Rozenberg and I. K. Schuller, **Decoupling electromagnetooptical responses by light in** $CdS/La_{0.7}Sr_{0.3}MnO_3$, in preparation

P. Salev, D. Sasaki, L. Fratino, S. Bag, M. Rozenberg, Y. Takamura, I.K. Schuller , **Magnetoresistance anomaly during electrical triggering of a metal-insulator transition**, in preparation

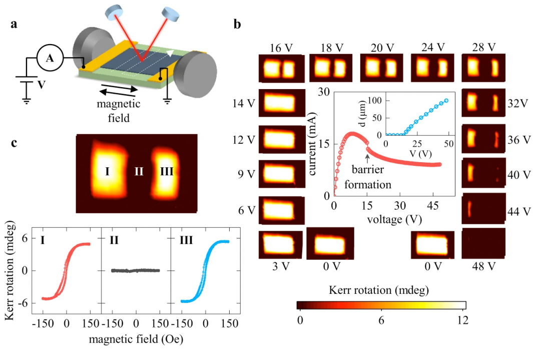

Figure 1: Schematic of the maximum Kerr rotation angle measurement (MOKE) setup. The magnetic field was applied in-plane along the device length. Voltage biasing was maintained without interruptions over the entire measurement time. b Simultaneously recorded I-V curve (center) and MOKE xy-maps (sides). The bright areas in the maps correspond to the ferromagnetic LSMO. In the maps, the electric current flows horizontally. As the I-V progresses through the NDR, a transverse insulating paramagnetic barrier appears in the device center and keeps expanding with increasing the applied voltage.

Study of Spin-to-charge conversion effect in ferromagnet/2DEG based nanodevices: The reading section of the MESO device

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Spin-orbitronic devices are capable of integrating memory and logic by combining ferromagnetism with spin-to-charge interconversion (SCI) property. This SCI is a vital property for the MESO device. The Magnetoelectric Spin-Orbit (MESO) technology [1] combines the advantages of the Magnetoelectric effect (ME) (input of the device) and Spin Orbit coupling (SOC) (read out part), to achieve an efficient SCI and the capability of storing non-volatile information in the magnetic state of the device. In this work, we focus on the MESO device's read-out part, using a 2-dimensional electron gas (2DEG) as a high SOC material [2]. The two principal advantages of using 2DEGs are the finite Rashba SOC they present, and the high tunability of their electronic structure, which is related to the Rashba-Edelstein effect (IREE) response [3]. The purpose of this section of the MESO device consists of applying a charge current through a ferromagnetic material, which is equivalent to the generation of the spin current via the ME effect, and this current will flow from the ferromagnet into the high SOC material. Due to the presence of IREE, which naturally appears in 2DEGs [4,5], the spin polarized current will be transformed into a charge current that will carry the information about the magnetization of the ferromagnet. In our study, we have designed, patterned and fabricated T-shaped nanodevices where the charge current is injected into a Co layer (the ferromagnet), and there it is transformed into a spin polarized current that will flow into the 2DEG, generating a perpendicular voltage output. Interestingly, we found signatures of SCC and studied its evolution as a function of the temperature, applied backgate, external magnetic-field or angle. Furthermore, since the current injected into the 2DEG is not a pure spin current, but a mixture of spin and charge currents (i.e. a spin polarized current), we tried to disentangle the IREE contribution from different spurious effects like Planar Hall Effect, Anomalous Hall Effect, etc. Our findings are very promising in terms of spin-logic approaches for alternative applications in computing field, paving the way towards a new generation of scalable, non-volatile and high energy efficiency beyond-CMOS spintronic logic devices.

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Multiferroïques

Multiferroics : past, present and prospects

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Multiferroics are a wonderful worldwide research subject due to their great application potential in the information industry, with, just to cite a few, multi-state information storage devices and new types of sensors. This enthusiasm of the community is clearly illustrated by the numerous books, articles and conferences on this subject (figure1):

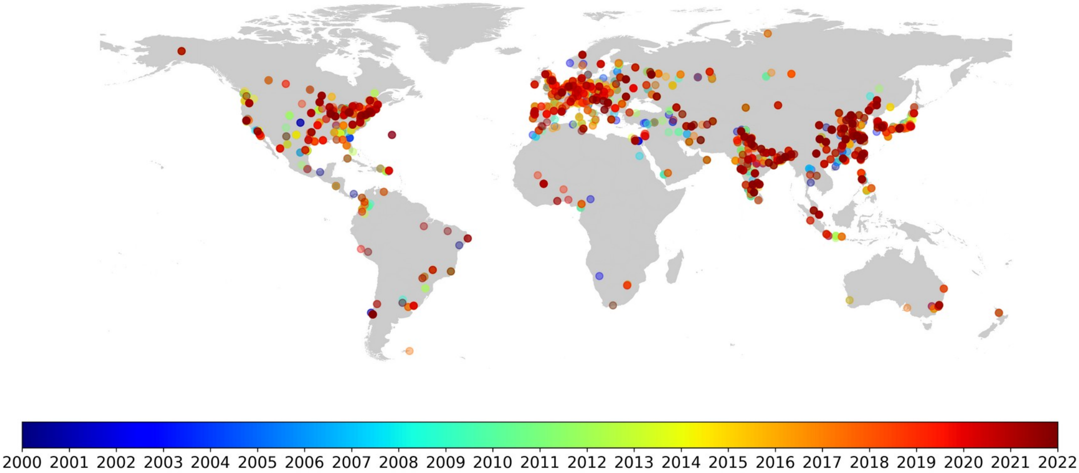

Figure 1 : Research publications on multiferroics since 2000

Multiferroics are a class of materials which was initially defined as the coexistence of more than two ferroic properties in a single phase, although the definition has been extended to include antiferroic properties. A coupling may exist between the orders, so that one property can be manipulated with the conjugate field of the other. As an example, magnetoelectric materials open up the profitable way to control magnetism by an electric field. The coexistence of electric and magnetic orders has been known for a long time, but in the last two decades, some key discoveries generated a lot of interest among researchers in this field and huge efforts have been devoted to the design and development of magneto-electric materials, majorly because of the need to limit energy consumption in electronics.

I will provide a general introduction to multiferroics, their history, the different mechanisms which support multiferroicity and the various paradigms which can be used for the conception of new multiferroic materials. I will give some prospects to try and answer the naive question: what next?

Chemical substitutions in '429' honeycomb antiferromagnets

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On the one hand, the honeycomb (HC) insulating antiferromagnets (AF) are attractive as candidates for showing quantum critical points between ordered and disordered magnetic phases [1] or for the new area opened by AF based spintronic [2]. On the other hand, searching for large magnetoelectric (ME) coupling, the linear ME (LME) AF compounds form a third class beside the type I and II multiferroics. Though these centrosymmetric LMEs are not multiferroics, a magnetic field application induces a polarization, with P proportional to H, as the prototype α-Cr_2O_3 AF corundum ($P\bar{3}c1$) [3,4] which structure contains HC layers.

This motivated the study of the $P\bar{3}c1$ LME $M_4Nb(Ta)_2O_9$ "429", with M=Mn^{2+} or Fe^{2+} or Co^{2+} [5], with crystal structures deriving from α-Cr_2O_3 that can be described as a stacking of two HC layers, a buckled one and a flat one, interconnected through face-sharing of their MO_6 octahedra (figure 1).

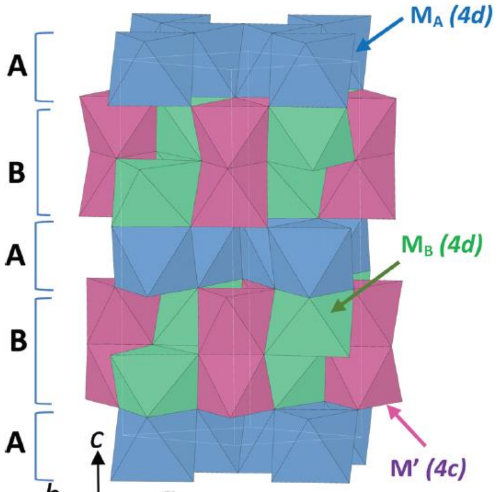

Figure 1: Schematic structure of the $M_4M'_2O_9$ compounds crystallizing in the α-Al_2O_3 structure ($P\bar{3}c1$). All the metal cations are in octahedral coordination, the M^{2+} cations being randomly distributed to build honeycomb layers [blue and green octahedra are for the M cations in the A and B layers, respectively, and the pink ones for the M'^{5+} cations].

As illustrated by doping diamagnetic cations to study the quantum spin liquid state in iridates [6], magnetic dilution was early shown to be an important way to bring quantum corrections to the staggered magnetization of AF. Considering the existence of several $M_{4-x}M''_xM'_2O_9$ solid solutions, the M'' dilution of the network formed by M magnetic cations can be exploited to produce enhanced physical properties. For instance, we have shown that the ME properties of $Fe_2Co_2Nb_2O_9$, $Fe_2Co_2Ta_2O_9$ and $Fe_3NiNb_2O_9$ [7,8,9] overpass those of $Co_4Nb_2O_9$ and $Fe_4Nb_2O_9$. Also, as compared to the latter, the $Ni_4Nb_2O_9$ paralectric 429 is unique as it adopts a derivated structure, cristallizing in *Pbcn* which is ferrimagnetic (FMI) below T_N=77K [10,11]. Interestingly, Zn for Ni substitution in $Ni_4Nb_2O_9$ allows to control magnitude of its negative magnetization below the compensation temperature T_{comp} (ref. [12] and figure 2).

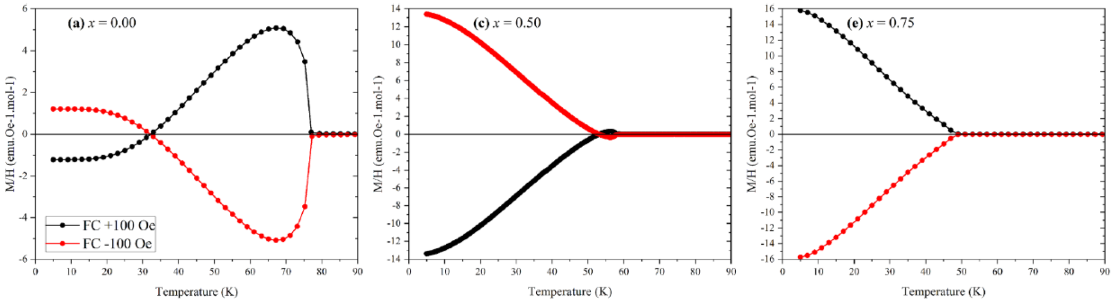

Figure 2: Magnetization versus temperature in FC mode for $Ni_{4-x}Zn_xNb_2O_9$ (H = +100 Oe, black curve and -100 Oe, red curve) from ref. [12]. For x=0.00 (a), T_{comp}=31 K and T_N=77K. For x=0.5 (b), a larger magnetization reversal is observed.

In this presentation, the substitution effect of paramagnetic and diamagnetic cations on the magnetic and LME properties of 429 compounds will be illustrated through several of our recent studies.

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Room temperature strained induced-ferroelectric switching in bismuth based perovskites

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Oxides have numerous applications in both electronics, spintronics and photovoltaics. The recent reports on the thin film growth of a new class of oxide perovskites, the bismuthates, brings new opportunities for electronic and spin-obitronic applications. However, most studies have so far focused on barium based compounds. Other members of the family have seen little interest, and their practical applications have not yet been investigated. Here we report that bismuthate $SrBiO_3$ can be grown as thin films by pulsed laser deposition. Following theoretical predictions, we have looked for a strain-induced ferroelectric state. Through piezoresponse force microscopy we will show that the films can display a ferroelectric behaviour at room temperature. Detailed atomic displacement mapping by scanning transmission electron microscopy suggests the presence of nanoscale strained and ferroelectric regions, coexisting with an unstrained and non-polar matrix. We will discuss the potential of our work for the development of oxide-based ferroelectric Rashba systems and on their potential for the ferroelectric control of spin-charge interconversion for beyond CMOS ultralow power computing.

Thermoélectricité

Recent advances and current challenges in thermoelectric materials

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Thermoelectric devices can achieve an "all-solid" conversion of electricity into a heat flow or of heat into electricity. They are commercialized as refrigerators or envisaged as localized electric generators to power wireless sensors for the Internet of Thing or to recycle the waste heat lost in industrial processes. Electrons act as the “fluid” carrying not only electric charge but also heat in the semiconducting materials that make up these devices. Their compactness and reliability compensate for their current low efficiency ($\leq$ 10%), which depends on the factor of merit *ZT* of the constituent materials, defined by the relationship: $ZT = \alpha^2 T/\rho\lambda$ with α the Seebeck coefficient, ρ the electrical resistivity and λ the thermal conductivity.

Several recent advances in thermoelectric materials rely on the democratization of electronic structure calculations and their close combination with experiments. To illustrate this, results on the ZrNiSn and NbFeSb half-Heusler compounds as well as the new $Mg_3Sb_{2-x}Bi_x$ series of materials will be presented. These two case studies will provide the knowledge base on thermoelectric materials and allow the introduction of concepts such as “defects engineering” and “multi-valley” transport. Then the presentation will move to PbTe and $Mg_2Si_{1-x}Sn_x$, where the concept of “band convergence” has been implemented to achieve Z*T* improvements. The introduction of a “resonant level” is another modification of the electronic structure upon doping which leads to increased *ZT* in thermoelectric material such as SnTe or MnTe.

An increase of Seebeck coefficient can be expected not only by a modification of the electronic structure but by a strong change in the scattering regime of the electrons upon “energy filtering” them. Finally, connections between thermoelectric materials and “topological insulators” will be attempted.

Phonons in complex crystals

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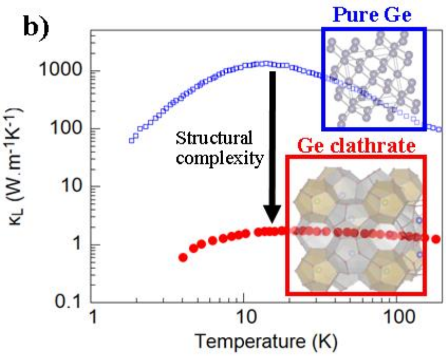
Exploiting the structural complexity of crystals at the scale of their unit cell is a well-established strategy in the search for efficient materials for energy conversion, which aims at disentangling and separately engineering heat and charge transport. Structural complexity, which can easily result in unit cells in the nanometer range that contain a large number of atoms of various types, is known to be an efficient way for designing thermal properties and the underlying phonon spectra. In the search for low lattice thermal conductivity in the field of thermoelectricity, one of the main strategies is the use of complexity at multiple length scales, from structural complexity within the crystal unit cell, to disorder, short range order, and nanostructuring. This route has resulted in the discovery of various complex crystals such as clathrates, tetrahedrites, skutterudites etc. with exceptionally low lattice thermal conductivity but essentially unaffected and tunable electronic properties. On the other hand, phonon measurements done in clathrates have revealed the existence of long-living acoustic phonons questioning the origin of their low lattice thermal conductivity ***[1]***. Another interesting case is that of High Entropy Alloys which exhibits a strong chemical disorder at the level of their unit cell leading also to a poor lattice thermal conduction. In this talk, I will first review spectroscopic measurements by means of neutrons and/or X-rays of the phonon spectrum and transport properties and the comparison with perturbative *ab initio* DFT calculation ***[2,3]***. We will see how the complexity acts on propagative phonons and is responsible for the anomalous behaviors in temperature of the lattice thermal conductivity without requiring the presence of strong anharmonicity or defects in clathrates ***[4]***. In a second part, I will introduce our recent measurements of phonons in High Entropy Alloys and show that these systems present a unique phonon dynamics at the frontier between fully disordered and ordered materials, characterized by long-propagating acoustic phonons in the whole Brillouin zone. W will see that the whole attenuation behavior can be understood in terms of scattering from force-constant fluctuations ***[5]***.



Impact of the structural complexity on the lattice thermal conductivity. Temperature dependences of the lattice thermal conductivity measured in pure Ge (blue points) and in a Ge-type I clathrate with composition $Ba_{7.81}Ge_{40.67}Au_{5.33}$ (red points)

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Texturation processing on thermoelectric silicide in a strong magnetic field

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We will present our recent results on silicide materials ($CrSi_2$ and $MnSi\gamma$) which were selected for their low cost and/or advantageous properties. For example, the Nowotny-chimney ladder compounds $MnSi\gamma$ ($\gamma \sim 1.73$) is particularly interesting as it exhibits sufficiently high ZT values (≥ 0.5 at 500 °C) in a wide temperature range, which is an advantage for stable electricity production. These advantages render them ideal candidates for the development of industrial prototypes. $CrSi_2$ is also an interesting p-type alternative materials with similar structural features to above mentioned one, and we will present here recent results on the improvement of its thermoelectric properties through a slip-casting process under a strong magnetic field.

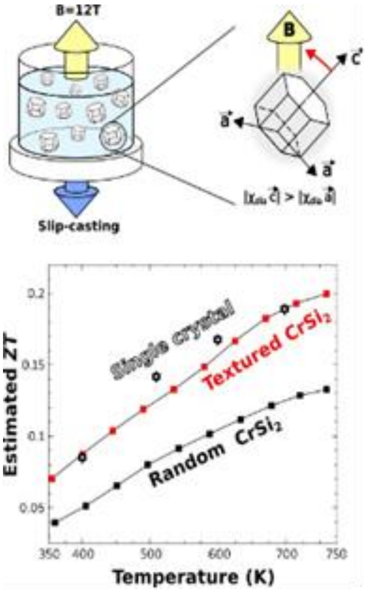

Figure 1: (above) Scheme of orientation of particles in suspension (below) Comparison of estimated zT for textured $CrSi_2$ and randomly orieneted $CrSi_2$ versus single crystal

25-25 janv. 2023

Matériaux solides pour le stockage et/ou la conversion de l'énergie

Fundamentals and current research trends in Solid Oxides Cells for energy production and conversion.

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Solid Oxide Cells (SOC) are ceramic devices that play a key role in the use of hydrogen as an energy vector. While operating in fuel cell mode, they offer an efficient way to convert the chemical energy contained in the H_2/O_2 redox couple into electrical energy and water. Conversely, in electrolysis mode, water vapor is converted into hydrogen, providing a storage option for surplus electricity. The promises of this cycle centered around H_2O, rather than CO_2, are driving the industrial and research efforts towards a clean and sustainable energy.

In this presentation the operation principles of the two most common SOC technologies, *i.e.* Solid Oxide Fuel Cells (SOFC) and Proton Conducting Fuel Cells (PCFC) will be introduced to understand the desirable properties of materials used in these devices. After a rapid introduction to the characterization technics used to evaluate the electrochemical performance of fuel cells and electrolysers, an overview of state-of-the-art cells and the current research axes to increase performance and decrease operation temperatures will be given.

Finally, the presentation will focus on the insights given by first principle calculations to understand the mechanisms at the heart of Solid Oxide Cells such as defect chemistry and ionic conduction, surface composition and catalytic activity or the relationship between the electronic band structure of oxides and their efficiency towards the Oxygen Reduction Reaction (ORR).

Gallia (Ga_2O_3) for Energy Electronics

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As most energy usage will be electrical (as well as transportation), the efficient management of electrical power is thus central to achieve the XXI century climatic goals. Ultra-wide bandgap (UWBG) semiconductors are at the very frontier of the electronics for energy management or *energy electronics*. A new generation of UWBG semiconductors will open new territories for higher power rated power electronics and solar-blind deeper ultraviolet optoelectronics. Gallium oxide - Ga_2O_3 (4.5-4.9 eV), has recently emerged pushing the limits set by more conventional WBG (~3 eV) materials such as SiC & GaN as well as for transparent conducting oxides (TCO).

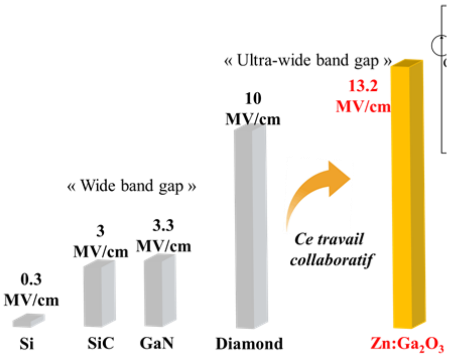
Physical properties of β-Ga_2O_3 thin-films will be discussed:

- An unexpectedly low 2D-like conductivity has been shown for n type Ga_2O_3 thin films which is resistant to high dose proton irradiation and largely invariant (metallic) over temperatures from 2 to 850K**.**

-we have showed the use of Ga_2O_3 electrodes has enabled, for the first time, an above-bandgap bulk photovoltaic effect on sandwich-like capacitors with transparent conducting electrodes (the architecture of solar cells) and under white light.

-We have demonstrated that Ga_2O_3 is also the native *p*-type TSO with the largest bandgap for any reported *p*-type TSO (e.g. NiO, SnO, delafossites, oxychalcogenides)**.**

- We have shown that doping with amphoteric Zinc a *p*-type β-Ga_2O_3 thin films shortens free carrier mean free path, resulting in the ultra- high critical electrical field of 13.2 MV/cm.[3] Fig.1Therefore, the critical breakdown field can be, at least, four times larger for the emerging Ga_2O_3 power semiconductor as compared to SiC and GaN.



Materials Today Physics 15 (2020) 100263

Thickness effect on vanadate TCO integrated on glass substrate using 2D nanosheets as a template

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$CaVO_3$ and $SrVO_3$ are novel transparent conductors, belonging to the group of perovskite oxides with strong electronic correlations [1]. This group of oxides also offers an important interplay between the structure of the material and the transport properties, impacting the optical properties through the modification of the charge carrier effective mass [2]. The technological potential of these new transparent conductors is largely related to the possibility of integrating vanadates on low cost substrates and especially on glass. In its amorphous form, vanadates are not conducting [3], imposing a growth approach keeping the crystalline character of the material. Recently, Boileau et al. demonstrated the possibility to integrate crystalline vanadate thin films with competitive properties by pulsed laser deposition thanks to $[Ca_2Nb_3O_{10}]^-$ nanosheets seed layer deposited onto glass substrate [4].

In this work, we study the effect of thickness on those films. The nanosheets seed layer allows to grow the films at a low thermal budget (500°C) required for the integration on glass. We show the evolution of electrical and optical properties using transport and spectroscopic analyzes. Additionally, we investigate the local electrical properties of the films by means of scanning spreading resistance microscopy (SSRM).

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Matériaux pour l'électronique du futur

Van der Waals epitaxy of two-dimensional transition metal dichalcogenides for spintronics

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Abstract

2D materials like transition metal dichalcogenides (TMDs) hold great promises for high performance and ultra-compact electronic, optoelectronic and spintronic devices. To date, most studies of TMDs have been performed on mechanically exfoliated flakes of micron size and their growth on wafer scale remains a challenge for the scientific community. In this presentation, after an introduction to 2D materials, I will demonstrate that molecular beam epitaxy (MBE) in the van der Waals regime allows for the growth on wafer-scale of single crystalline TMDs down to the 2D limit. MBE grown TMDs exhibit comparable electronic properties as mechanically exfoliated flakes. In the field of spintronics, TMDs offer interesting properties such as large spin-orbit coupling (in WSe_2 or $PtSe_2$), various symmetries (1H, 1T or 1T'), electrically tunable electronic properties and more recently ferromagnetic properties. In this prospect, I will present some emerging materials and spintronic devices based on TMDs.

Direct visualization of Rashba-split bands and spin/orbital-charge interconversion at $KTaO_3$ interfaces

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The two-dimensional electron gas (2DEG) at the interface between $SrTiO_3$ (STO) and $LaAlO_3$[1], displays a wide array of functionalities; such as high electronic mobility, low temperature superconductivity,[2] and tunable Rashba spin-orbit coupling (SOC)[3]. Among these, the Rashba SOC enables gate tunable highly efficient spin – charge interconversion which paves the path towards spin-orbitronics[4]. Along with the experimental observation of record spin Edelstein length in STO based 2DEGs[4], it has also been predicted theoretically that the orbital Edelstein effect exceeds the spin Edelstein effect by more than one order of magnitude in this system[5].

Similar to STO, $KTaO_3$ (KTO) is a quantum paraelectric material where due to the presence of Ta (5d element), the Rashba SOC in this 2DEG is expected to be larger than STO 2DEGs. In this work, 2DEGs are generated by the deposition of Al metal on KTO single crystals. Transport and spin-pumping measurements are performed to explore the 2DEG properties and the spin Edelstein effect, respectively[6]. Further, the samples are characterized by angle-resolved photoemission spectroscopy to probe the band structure[7]. In addition, the band resolved spin and orbital Edelstein effects have been computed and we predict that these efficiencies exceed by at least twice than the other oxide 2DEGs[7].

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Mn_3X (X=Sn, Ge) non-collinear antiferromagnets

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Mn_3Sn and Mn_3Ge order antiferromagnetically well above room temperature. At room temperature, they display a large Anomalous Hall Effect (AHE) whose sign can be inverted with a small (< 0.1 T) magnetic field. The combination of room temperature and small magnetic field makes this material promising for applications. Following the discovery of room-temperature AHE [1], numerous interesting properties have been discovered, which are all detectable at room temperature. The list includes thermoelectric (Nernst) and thermal counterparts of AHE [2,3], skyrmionics domain walls with memory [4], field-induced twist of spin texture [5], large piezo-magnetism [6] as well as its magnetostrictive [7] counterpart.

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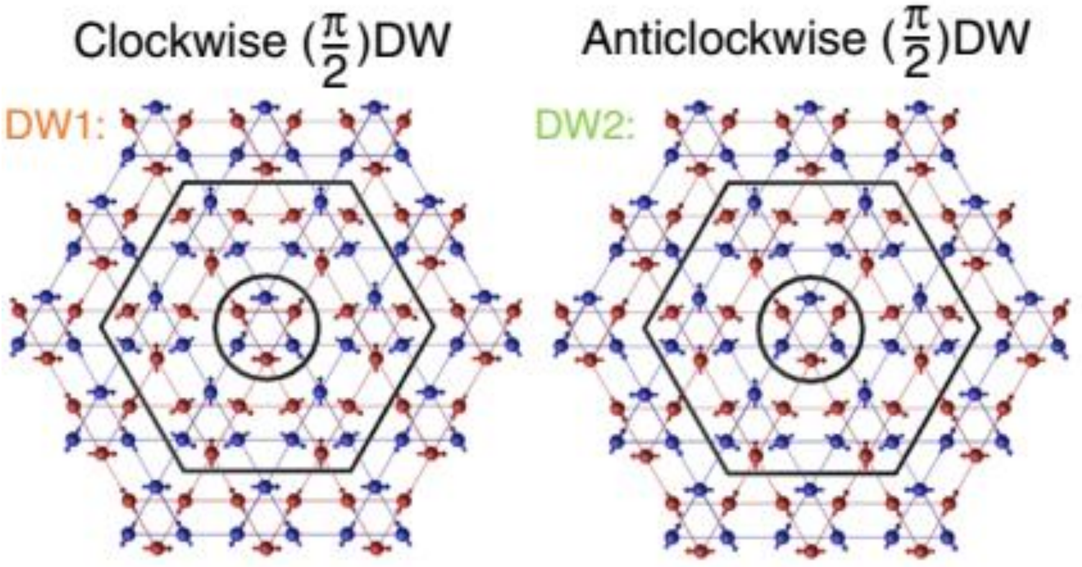

Effect of Metallic reservoir on phase transitions in strongly correlated systems

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Mott insulator materials are interesting for neuromorphic devices, such as artificial spiking neurons[1]. Several order of magnitude change in the resistivity across the metal to Mott insulating transition(MIT) of Mott insulators can be exploited in artificial neuromorphic devices. Controlling of MIT in Vanadium Oxide is possible in hybrid heterostructurescite of thin-film the material and photoconductive semiconductor Cadmium Sulfide(CdS) with the light [2]. Despite VO_2 and V_2O_3 MITs being similar, the behavior of metal-to-insulator(MIT) with CdS illumination is dramatically different. The illumination suppresses the T_{MIT} of V_2O_3, which is quickly pushed down toward zero temperature. While the light illumination minor effect on T_{MIT} of V_2O_3.\\

To understand the experimental behavior, we theoretically model these systems. The CdS, in these heterostructures, is modeled as incoherent metallic reservoirs coupled to the Vanadate thin film and illumination strength is modeled as the coupling strength(Γ) between them.These Models are solved using Dynamical Mean Field Theory(DMFT) with CTQMC asan impurity solver. Qualitatively, the Hubbard model(HM) could capture the suppression of MIT observed in V_2O_3. In contrast, the results for VO_2 point to the possible relevance of the structural change.

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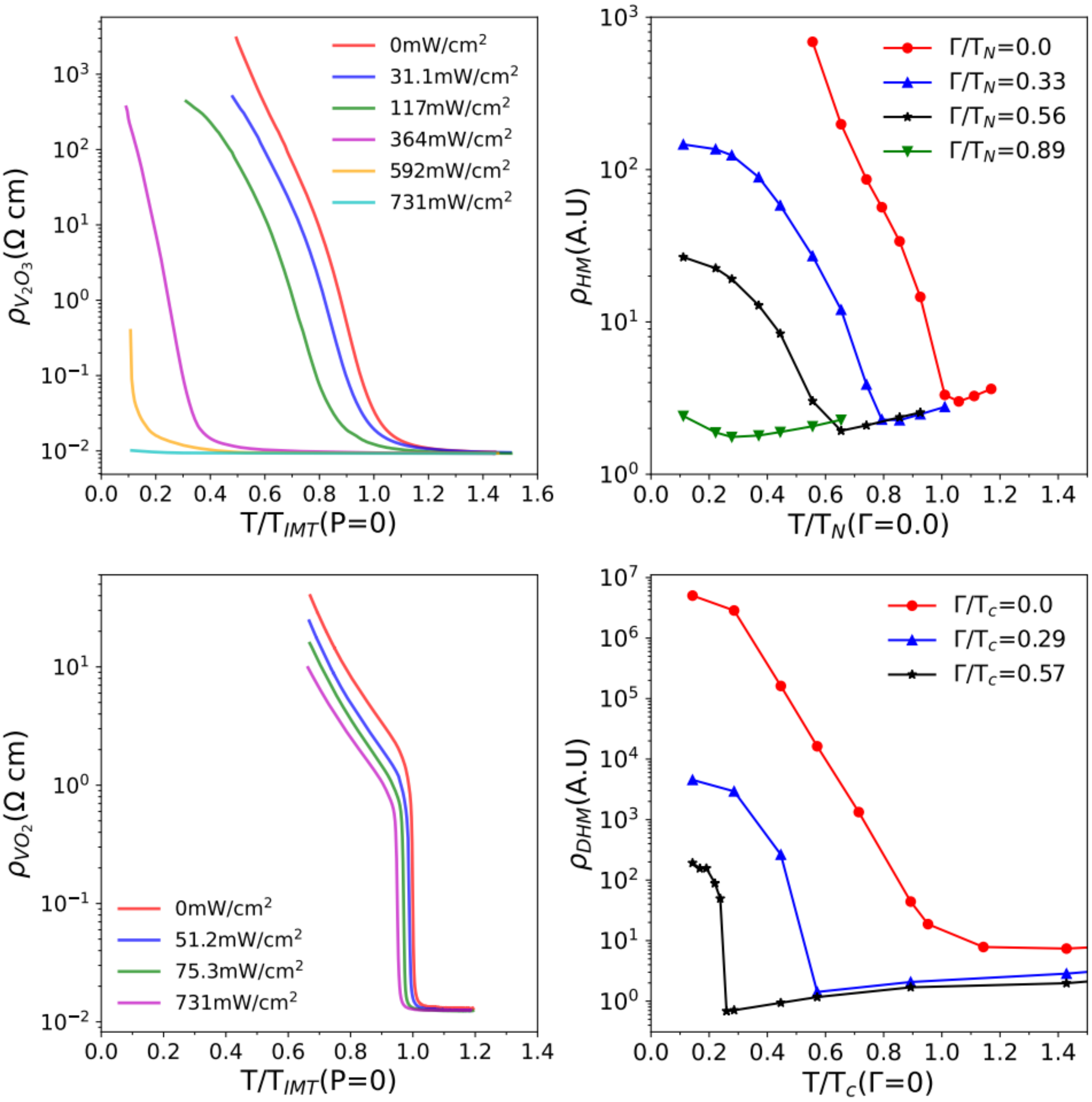

Fig: Experimental result of resistivity(ρ_{V2O3})as a function of Temperature(T) for various light illumination power(P) in CdS/V_2O_3 (Top-right) resistivity(ρ_{HM}) of Half filled Hubbard model as a function of Temperature(T) for various values of coupling strength(Γ). (Bottom-left) Experimental result of resistivity(ρ_{VO_2}) as a function of Temperature for various light illumination power(P) in CdS/VO_2 (Bottom-right) Drude resistivity(ρ_{DHM}) of half-filled Dimer Hubbard model(DHM) as a function of Temperature(T) for various values of coupling strength(Γ)

Multiferroïques

Voltage-controlled magnonic crystal in oxide heterostructures at the sub-micron scale

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Magnonics where magnons, the associated quasiparticles of spin waves are used to perform advanced logical or analogue functions represents a promising paradigm for new means of information processing for beyond complementary metal oxide semiconductor (CMOS) based architectures. Furthermore, in view of the emerging nano-magnonics which can eventually lead to a large-scale integration of magnonic devices new approaches for a compact, reconfigurable operation of magnonic device are required. Although such a reconfigurability is key to any efficient application such as magnonic filters, it has hitherto only theoretically [1] but not experimentally been shown on a sub-micron scale. On the other hand, multiferroics inherently offer compact means to implement voltage-control and reconfigurability in such microscopic magnonic systems [2]. In this work, we combine multiferroics with ferromagnets by employing a fully epitaxial heterostructure to achieve such voltage-controlled and reconfigurable magnonic system. Frequency filtering is most often based on magnonic crystals (MC) where a periodic modulation of the spin wave's energy landscape results in frequency bandgaps in the magnon spectrum [3,4]. Here, we employ a thin-film multiferroic bismuth ferrite $BiFeO_3$ (BFO)-lanthanum strontium manganite $La_{2/3}Sr_{1/3}MnO_3$ (LSMO) heterostructure ($\alpha^{\mathrm{Gilbert}}{}_{\mathrm{LSMO}}{\sim}6 \cdot 10^{-3}$). Instead of modulating the sample shape, we create a MC by imprinting a periodic remnant electrical polarization in the multiferroic BFO layer which modulates the effective magnetic field in the ferromagnetic layer. We characterize the spin wave propagation spectra in this artificial, voltage-induced magnonic crystal and demonstrate the occurrence of a robust magnonic bandgap with >20 dB rejection, i.e. filtering. The imprinted ferroelectric domains can be reconfigured repeatedly and are long-lived.

Our results open a new path for the transduction and configurable filtering of spin waves within a single magnonic device. In general, by bridging between the scientific fields of functional oxides and magnonics, it opens new perspectives for the development of beyond CMOS based technologies [5].

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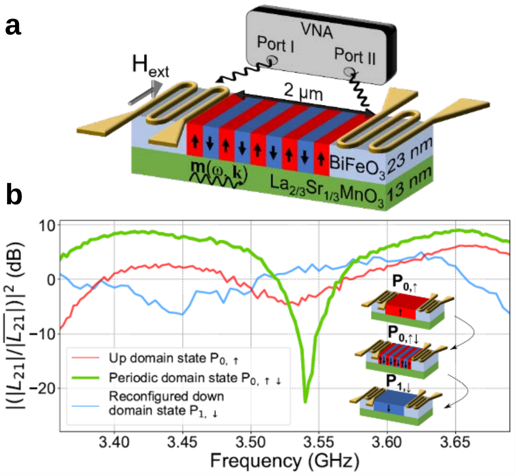

Fig. 1 : ***a*** *Experimental setup with periodic BFO domains* ***b*** *Evidence for the bandgap for the BFO/LSMO heterostructure with periodic domains in the BFO. Pn,m label the different domain states where n is the cycle number (1 cycle: down (virgin) → up → periodic) and m the direction of the ferroelectric polarization.*

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*all authors contributed equally

Tuning the multiferroic properties of $BiFeO_3$ under uniaxial strain studied by Raman spectroscopy

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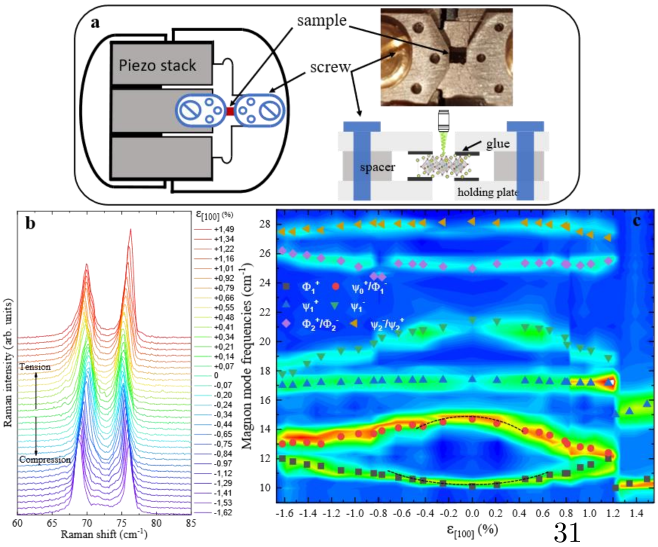
More than twenty years ago, multiferroic compounds combining in particular magnetism and ferroelectricity were rediscovered. Since then, $BiFeO_3$ (BFO) has emerged as the most outstanding multiferroic by combining at room temperature almost all the fundamental or applicative properties that may be desired as for example: electroactive spin wave excitations called electromagnons, conductive domain walls or a low bandgap of interest for magnonic devices, low-energy spintronic and photovoltaics. All these properties have so far only been discontinuously strain engineered in thin films according to the lattice parameter imposed by the substrate. In this study, we have explored the ferroelectricity and the dynamic magnetic response - cycloidal antiferromagnetic order - of BFO bulk under uniaxial strain.

Using elasto-Raman spectroscopy combined with effective Hamiltonian calculations, we demonstrate that the polarization magnitude is enhanced under tensile strain. The magnonic response is entirely modified, low energy magnon modes being suppressed for tensile strain pointing out a transition to an homogeneous magnetic state. The energies of both polar modes and several spin excitations are to the square of the strain at low deformation and linear at higher strain. Finally, we reveal that uniaxial tensile strain applied on BFO bulk allows a differentiated modification of its polarization and a 2D transformation of the magnetic structure.



a. Scheme of uniaxial strain cell

b. Phonon spectra measured for several compressive and tensile strain inside the pressure cell

c. Magnon modes frequencies and 2D colormap of the Raman intensity (color scale) as a function of the deformation $\varepsilon_{[100]}$

Magneto-electric properties of spin ices

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The pyrochlore lattice featuring corner sharing tetrahedra has been a playground for magnetic frustration effects . An example of exotic phases that may emerge is the so called spin ices – as referred to water ice with its O-H bonds – where, on each tetrahedron, two spins point inward and the other two point outward. This is a highly degenerate state and can be viewed as a liquid of magnetic spins with peculiar short range correlations. Out of this equilibrium state, an excitation may be produced when one spin in one tetrahedron is reversed, creating a "magnetic monopole". Quite recently, a model due to Khomskii has suggested that this magnetic monopole may carry an electric dipole [1] opening the route towards new magneto-electric effects and multiferroicity in spin ices and related phases. Up to now, very few experimental evidences exist [2]. Here, we present extensive results obtained on two different compounds: the classical spin ice $Ho_2Ti_2O_7$ and the quantum spin ice $Tb_2Ti_2O_7$. We show that, at temperatures as high as 100K, pyro electric currents are measured, associated with flowing electric charges arising from thermally activated defects. These effects are not sensitive to magnetic field. On the contrary, magneto-electric effects are observed below typically 20K, that are noticeably different in the Ho and Tb compounds. These experimental results will be compared to classical Monte-Carlo simulations of the Khomskii model and discussed in the framework of magnetic monopoles and their possible electric moment.

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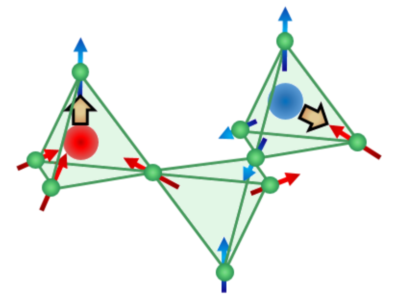

Magnetic and electric configurations on the pyrochlore lattice with two monopoles

Thermoélectricité

Ab initio description of electron-phonon and phonon-phonon scattering processes in density functional theory for the calculation of charge and heat transports

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The future sparsity of carbon-based fuels, the increasing energy cost, together with the growing concern of society over environmental problems, make the performance improvement of energy conversion devices – thermoelectricity, photovoltaics – a topic of high importance. Such devices are mainly designed by using macroscopic models -the drift-diffusion for electronic transport, or the Fourier formalism for heat/energy transport- which assume local equilibrium and simplified (averaged) material properties for the carrier relaxation times. Huge progress has however been achieved in the description of scattering processes with methods based on the density functional perturbation theory (DFPT). We will show that electron transport characteristics of bulk semiconductors are well described within the approach that couples DFPT electron-phonon scattering rates with the semi-classical Boltzmann transport equation (BTE), and the same is true for phonon-phonon scattring rates for the thermal conductivity, with bismuth as an example. We will also discuss the electron and phonon coupled equations for thermoelectricity as well as the effect of nano-structuring.

Acknowledgements:
Calculations have been performed using the QUANTUM ESPRESSO[1] and EPW[2] softwares. We acknowledge access to high performance computing (HPC) resources by the Partnership for Advanced Computing in Europe (PRACE Project No. 2019204962), by the French HPC centers of TGCC, CINES and IDRIS (GENCI Project 2210) as well as to the 3L-hpc local computer cluster partly supported by the DIM SIRTEQ (région Île de France) and École Polytechnique. Financial supports are also acknowledged: CEA ANCRE program (project Thermoint), Labex Nanosaclay ANR-10-LABX-0035 (Flagship project MaCaCQu), and ANR-21-CE50-0008 (project Placho).

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Experimental study of spinon phonon coupling in spin chain cuprates

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Romuald Saint-Martin[1], Rolf Heid[3], Alexandre Ivanov[4], Andrea Piovano[4],
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The thermal properties of spin liquids and more generally of unconventional magnets attracted much attention over the last decade. For instance, cuprate spin chains, such as $SrCuO_2$ Sr_2CuO_3 and Ca_2CuO_3, exhibit amazing heat transport properties, with an exceptionally high magnetic contribution to the heat conductivity κ along the spin chains. Current interpretation assumes that this heat flow is carried by spinons, the fractionalized magnetic excitations typical of the 1D antiferromagnetic Heisenberg model. κ is thus a direct manifestation, at a macroscopic scale, of the quantum nature of those 1D chains [1]. These thermal properties are also accompanied by a hidden fragility, as a small perturbation of the spin chain, as for example non magnetic substitution at the Cu sites, may interfere with, and eventually hinder, the magnetic contribution to heat transport [2]. Furthermore, κ rapidly drops above 50 K, a behaviour likely due to growing scattering rate of spinons by phonons. To shed light on this issue and constrain experimentally the spinon-phonon coupling, we have studied the phonon dispersions in these materials, by means of inelastic neutron scattering, to determine whether they exhibit anomalous behavior as a function of temperature and/or upon crossing the spinon spectrum. We come to the conclusion that there are no obvious anomalies in the phonon dispersions, which suggests a weak spinon-phonon coupling regime [3]. These results support a recent theoretical work by Chernyshev *et al.* [4] who derived a microscopic spin-phonon scattering rate where phonons act as thermally populated defects for the fast spin excitations. In this approach, only a weak coupling constant is necessary to explain $\kappa(T)$, unlike previous scenario calling for the strong coupling limit.

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Systematic study of $Ag_2Te_ySe_xS_{1-x-y}$ chalcogenides for wearable thermoelectrics

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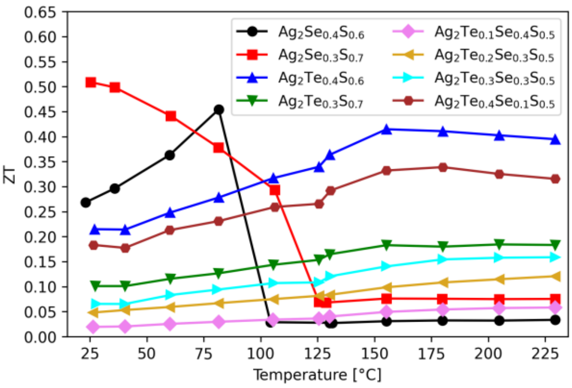
Wearable renewable energy generators are an attractive alternative to battery-based systems and can generate power up to a few Watts for portable electronic equipment. Although the most inorganic semiconductor materials are brittle at room temperature (RT) the $Ag_2Te_ySe_xS_{1-x-y}$ chalcogenides show exceptional plastic deformability and high thermoelectric performance making them suitable materials for wearable thermoelectrics.



A series of samples was prepared by rapid casting: $Ag_2Te_ySe_xS_{1-x-y}$ (with x, y, x or y = 0.1; 0.2; 0.3; 0.4.) in to form of Ø = 3 mm, 12 mm long homogeneous ingots. Significantly high ZT ≈ 0.5 at RT was measured for $Ag_2Se_{0.3}Se_{0.7}$ compound. $Ag_2(S+Se)_1$ and $Ag_2(Se+Te)_1$ ternary systems at RT crystalize in an orthorhombic or monoclinic structure, depending on the detailed S/Se, Se/Te atomic ratio. Addition of Te into these systems is introducing favorable cubic phase, as well observed in $Ag_2(S+Te)_1$ ternary middle region. Well known monoclinic – cubic phase transformation of $Ag_2(S+Se)_1$ is pulled down to lower temperatures (even under RT) where it stabilizes with rising Te concentration. Highly disordered Ag+ ions stay present in the cubic phase mimicking amorphous structure (examined by diffraction) causing low thermal conductivity.

In this contribution, we present a systematic study of $Ag_2Te_ySe_xS_{1-x-y}$ chalcogenides. Temperature induced structural phase transformations are examined by differential scanning calorimetry and synchrotron in situ diffraction. Inelastic neutron scattering investigations shed light on the compounds' phonon properties showing a phonon renormalization and broadening with addition of Se/Te to Ag_2S and temperature treatment. The results are supported by density functional theory and molecular dynamics calculations. We present data from thermoelectric characterizations carried out from RT up to 230°C.

Posters

$(Cr_{1-x}V_x)_2O_3$ Mott transition driven by electric-pulses for artificial neural network and data storage applications

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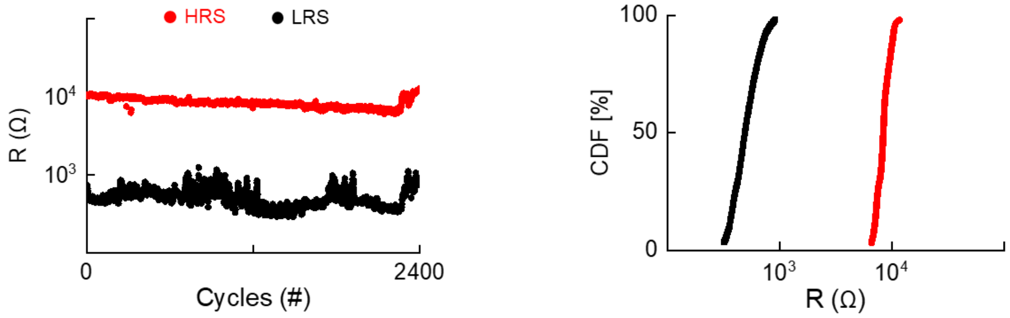
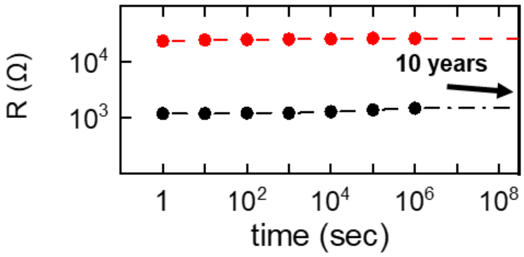
Resistance random-access memory (RRAM) is considered as a promising candidate to replace the flash memory technologies that approach their limits due to miniaturization and short economical payback [1]. In that context, canonical Mott insulator such as $(Cr_{0.30}V_{0.30})_2O_3$, or AM_4Q_8 have shown a surge of interest as they can reproduce the writing-erasing processes of memory devices thanks to a reversible non-volatile Insulator-to-Metal transition (IMT) triggered by electric pulses [2-3]. Previous studies have demonstrated competitive memory performances in Mott insulator thin films but so far these studies overlooked the variability of the devices [4]. Here we investigate the resistive switching in Mott insulators thin films of $(Cr_{1-x}V_x)_2O_3$ (x = 0.7) integrated in micro-sized memory cells and report for the first time the cycle to cycle variability and retention time of the high and low resistance states. To this end, thin films were deposited and annealed in order to reach the expected stoichiometry and a good crystalline quality. The electrical behavior was investigated on MIM structures using 2 µm via memory cells made of 50 nm thick $(Cr_{0.30}V_{0.70})_2O_3$ Mott insulator thin films. Preliminary experiments on these devices using short electric pulses for the SET and RESET show an endurance of more than 2000 times (Figure 1.a). The cumulative distribution function (CDF) curve demonstrates an average R_{OFF}/R_{ON} ratio close to 20 (Fig 1.b). Moreover, both R_{OFF} and R_{ON} resistance states exhibit a very good temporal stability at room temperature and the retention time can be extrapolated up to 10 years (fig 1.c). This work show therefore the potential of $(Cr_{0.30}V_{0.70})_2O_3$ Mott insulator thin films for integration into the next generation of non-volatile memories and multi-level cell.



(a) *(b)*



(c)

Fig1. (a) Cycling endurance obtained on a device of 2 µm via and 50 nm thick $(Cr_{0.3}V_{0.7})_2O_3$ demonstrator showing 2400 resistive switching cycles. (b) Resistance distribution for the high (HRS) and low (LRS) resistive states.(c) Data retention at room temperature extrapolated to 10 years for HRS and LRS.

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A Verwey-like transition in multiferroic gallium ferrite thin films

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Temperature dependent X-ray absorption spectroscopy and X-ray magnetic circular dichroism experiments were performed at the Fe $L_{2,3}$ edges to unveil the magnetic orbital moment and spin-orbit coupling (SOC) behaviour in thin films of the multiferroic $Ga_{0.6}Fe_{1.4}O_3$ (GFO) compound. A thorough analysis of the data evidenced a non-monotonous behaviour for both magnetic orbital moment and SOC with a minimum at approximately 120 K, accompanied with indications of disturbances of the magnetic exchange and electric field dipole. REsonant PhotoEmission Spectroscopy (RESPES) experiments performed at the Fe $L_{2,3}$-edges rendered an important modification of the crystal field configuration around this temperature value, pointing at a temperature-driven structural trigonal distortion. These instabilities can be compared to those observed in other iron oxides, in particular during transitions such as the Verwey transition, with the difference that on GFO they do not have any impact on the macroscopic magnetic properties, such as the coercive field and the global magnetization. This work demonstrates that the absence of instabilities in magnetism at the macroscopic scale does not grant for the absence of atomic-scale fluctuations. Such atomic-scale fluctuations of the SOC are undoubtedly shown here and have an impact on the spin Hall magneto-resistance response of the films. This point is of importance for prospective applications of GFO in spin-orbitronics.

Absence of superconductivity in bulk layered Ni^{1+} doped nickelates

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The discovery of superconductivity below $T_c \sim 15$ K in doped infinite layer $Nd_{1-x}Sr_xNiO_2$ nickelate thin films on $SrTiO_3$ substrates in 2019 has generated an enormous interest in the condensed matter community because of their great similarities with cuprates [1]. Then, superconductivity was also found with maximal T_c reaching 20 K, using other rare earth or alkaline earth doping elements, such as La,Sr (or Ca) [2,3] and Pr,Sr [4] based systems and on a different substrates $(LaAlO_3)_{0,3}(Sr_2AlTaO_6)_{0,7}$ [5,6].

In our laboratory, we have studied the analogous bulk materials of such systems. We have synthesized good quality polycrystalline samples of Sr doped $(Nd_{1-x}Sr_x)NiO_2$, $(Pr_{1-x}Sr_x)NiO_2$ up to $x = 0.2$ and Ca doped $(Nd_{1-x}Ca_x)NiO_2$ series up to $x = 0.5$. Physical measurements carried out on these systems revealed no superconductivity in any of these compounds so far, but a spin-glass like (below T*) and insulating behaviour at low temperature was observed (Fig. 1).

We also synthesized a new polycrystalline phase $NdNiO_{2+y}$, a partial reduced form of $NdNiO_3$. Although its powder X-ray diffraction (XRD) pattern looks very similar to the one reported by Moriga et al. [7], the crystal structure we found by Transmission Electron Microscopy (TEM) is totally different. The Selected Area Electron Diffraction (SAED) evidenced a modulated structure in a tetragonal subcell with the parameters $a \approx 3.8$ Å and $c \approx 3.5$ Å. Due to the commensurate nature of the modulation, the structure can be described in a monoclinic supercell with the parameters $a \approx 16.4$ Å, $b \approx 7.8$ Å, $c \approx 5.5$ Å and $\gamma \approx 105°$ (Fig. 1). A first structural model has been determined using 3D electron diffraction crystallography and has been refined from powder XRD data. The full determination of oxygen positions, as well as the physical properties studies are still under progress.

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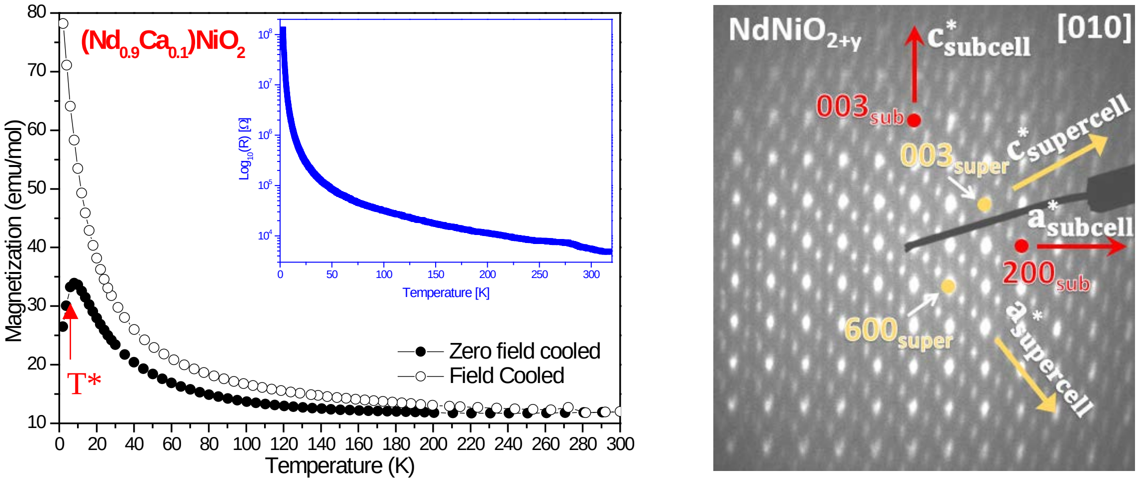

Fig.1 ***Left:*** *Magnetization of* $Nd_{0.9}Ca_{0.1}NiO_2$ *pellet from 300 K down to 2.5 K in applied field of 100 Oe (with T* ~ 10 K). Inset: its electrical resistance in the 2.5 - 320 K range.* ***Right:*** *TEM [010] SAED pattern of* $NdNiO_{2+y}$.

Antagonism between polar displacements and Rashba phenomena in strained $SrTiO_3$

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Spintronic exploits the spin degree of freedom in addition to the charge of carriers, yielding numerous applications in data storage for instance [Nat. Mater. **6**, 813 (2007)]. An alternative pathway toward lower power spintronics exists and exploits the spin-orbit interaction (SOI) of non-magnetic materials through the Spin Hall Effect (SHE) [Phys. Lett. **13**, 467 (1971); Science **306**, 1910 (2004)] and inverse Spin Hall Effect (ISHE) Nat. Commun. **3**, 629 (2012); Phys. Rev. Lett. **96**, 246601 (2006)]. More recently, a promising pathway toward efficient spin-charge current interconversion has been identified and uses a peculiar interplay between polar displacements and SOI: when inversion symmetry is broken, such as at interfaces, surfaces or in ferroelectric compounds, the polar displacements can yield a Rashba interaction lifting the degeneracy of bands according to their spin [JETP Lett. **39**, 78 (1984)]. The efficiency of the conversion is related to the Rashba parameter, usually assumed to depend directly on the spin-orbit interaction and polar displacements amplitude.

In this study, $SrTiO_{3,}$ a prototypical compound allowing Rashba phenomena [Nat. Mater. **15**, 1261 (2016)], is used for studying the interplay between polar displacements and Rashba interaction on the basis of *first-principles* Density Functional Theory simulations. Within ferroelectric phases reached under compressive strain, an unexpected suppression of Rashba effects when polar displacements amplitude increases is observed. By inspecting the role of individual lattice distortions, this surprising behavior is ascribed to the suppression of Ti t_{2g} orbital degeneracies induced by the polar displacements. In turn, it weakens the spin-orbit interaction amplitude and hence Rashba effects. This antagonism observed in $SrTiO_3$ thus highlights that a large electric field is not necessarily a prerequisite for reaching a sizable Rashba parameter and that the latter quantity might be bounded to a upper value.

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Charge ordering as the driving mechanism for superconductivity in rare-earth nickel oxides

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Superconductivity is one of the most intriguing properties of matter characterized by zero electrical resistance and perfect diamagnetism. Its origin can be understood on the basis of an attractive interaction that bounds electrons into Cooper pairs. The most widely studied superconductors are the perovskite cuprates which have the highest critical temperature (T_c) at ambient conditions. In the search for compounds analogous to cuprates, nickel oxides were long proposed to host superconductivity [1,2]. This research crystallized in 2019 with its discovery in infinite layer nickelates $R_{1-x}Sr_xNiO_2$ [3] and lately in a reduced Ruddlesden-Popper $Nd_6Ni_5O_{12}$ [4] with similar critical temperatures (T_c=9-15 K), albeit without clarifying the pairing mechanism.

Here we use Density Functional Theory (DFT) to show that superconductivity is tightly related to a charge and bond ordered state that produce a significant electron-phonon coupling. We reveal the existence of an unstable 1.5+ formal oxidation state (FOS) of Ni cations ($3d^{8.5}$) in the half-doped case that prefers to transform to more stable 1+ ($3d^9$) and 2+ ($3d^8$) FOS in the ground state. It results in a bond disproportionation of O_4 groups, a charge ordering and an insulating state. Starting from this half doped situation, doping is shown to suppress disproportionation effects, ultimately resulting in a metallic regime. Once this charge ordered state is suppressed, the related bond disproportionation mode is still highly coupled to the electronic structure and the resulting electron-phonon coupling is sufficient to explain the T_c dome versus doping content observed experimentally. It suggests that the vicinity of a charge ordered state is a prerequisite for superconductivity in the nickelates. Hence, these compounds appear more similar to bismuthates than to cuprates [5].

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$Co_3Sn_2S_2$, a kagomé semi-metallic half-metal

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$Co_3Sn_2S_2$ becomes ferromagnetic below ~175 K. The spins align perpendicular to the kagomé planes. It displays a large anomalous Hall effect [1] as well as its Nernst [2] and thermal Hall [3] counterparts. Thanks to the low density of carriers, mobility is high and quantum oscillations are easily detectable [3]. Among a variety of interesting properties, one can mention a very broad window of critical fluctuations [4], most probably driven by the smallness of the Ginzburg number in this semi-metallic itinerant magnet.

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Combined in situ (T, P, E) SC-XRD analysis of a magnetoelectric plastic-crystal

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Materials presenting a coupling between two ferroic orders, such as ferroelectricity and (anti)ferromagnetism, are of particular interest owing to their high potential for applications in memory devices [1]. Therefore, there is an important research effort to design new multiferroic materials with improved magnetoelectric coupling. Molecule-based materials are particularly appealing to achieve magnetoelectric coupling since the versatility of each molecular components offers the possibility to tune the physical properties [2]. On the other hand, plastic crystalline molecular materials have attracted significant interest in the past few years because the solid-solid phase transition from the ordered crystal phase to the disordered plastic-crystal phase (PC) is generally accompanied by large enthalpy/entropy variations [3]. Recent investigations have been carried out on so-called ferroelectrics PC where the PC-crystal transition is associated to the para-ferroelectric transition giving rise to barocaloric, electrocaloric and multicaloric effects [4].

The ferroelectric PC triethylmethylammonium tetrabromoferrate (III) reported in 2012 by H. Chai et al [5] is particularly attractive as the para-ferroelectric transition, taking place around 355K, is accompanied by a change in the magnetic properties. At room temperature, $[(Et_3NMe)^+(FeBr_4)^-]$ crystallizes in polar space group $P6_3mc$ and presents a structural transition leading to a new ferroelectric phase around 170K. More recently, we observed a color change from dark red to yellow as function of temperature. The structural properties at the origin of this wide range of physical properties, especially the ferroelectricity, are almost unexplored. Indeed, $[(Et_3NMe)^+(FeBr_4)^-]$ shows an important disorder, complicating the atomic structure determination of the cationic part. To overcome these difficulties, we investigated the structural behavior of this compound by *in situ* X-ray diffraction in different non-ambient conditions. First, we explored the phase diagram from room temperature to 5K and we quenched the room temperature phase at low temperature. Then, we performed *in situ* SC-XRD under pressure from ambient pressure to 4.5 GPa. Both experiments, at low temperature and under pressure, evidence an absence of correlation between the structural phase transition and the color change. Finally, thanks to the new experimental setup we develop in our lab, we realized an *in situ* SC-XRD under a static electric field of 2kV/mm. All these non-routine measurements allowed us to have a better description of the cationic part disorder of $[(Et_3NMe)^+(FeBr_4)^-]$. This is a first step to establish structure-properties relationships of this multifunctional material.

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Core-level photoemission in Li_xCoO_2 below the surface

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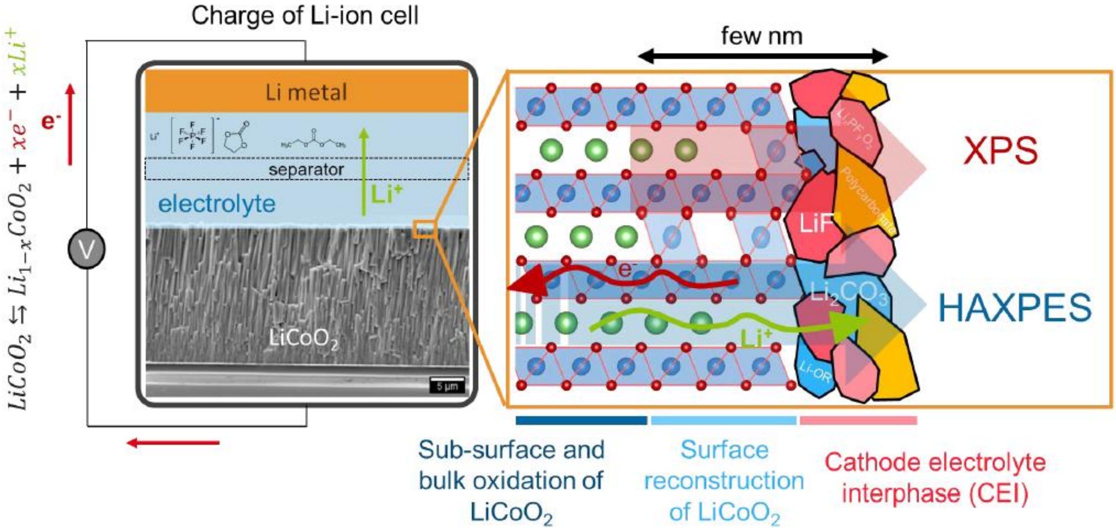
Photoemission measurements are particularly surface-sensitive, with a sampling depth of the order of a few nanometers for soft X-rays. This typically corresponds to the thickness of the solid-electrolyte interphase that can be created during cycling of battery active materials, or to that of surface alterations. In this poster, we present our experimental setup combining soft and hard X-rays to probe the surface versus bulk electronic structures, and discuss measurements on Li_xCoO_2, a prototypical material for the positive electrodes of lithium-ion batteries.



Deep Learning Hamiltonians from Disordered Image Data in Quantum Materials

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Current advancements in surface probes have allowed researchers to have a large availability of images of quantum materials over different lengths and time scales. Those images have revealed the formation of intricate patterns as some materials approach criticality. In such cases, the spatial structure should encode information about interactions, dimensionality, and disorder – a spatial encoding of the Hamiltonian driving the pattern formation.

With the well-known capabilities of deep learning techniques for image recognition, we have developed a framework to recognize the underlying physics that best describes the complex pattern formation in a film of VO2 during the metal-to-insulator transition.

In this poster, we will go through the steps in developing the deep learning model: the selection of the Hamiltonians and the patterns they form, the data preparation, and the multi-label classification of images using a Convolutional Neural Network. We then vet this procedure using SNIM maps. Finally, we apply this method to new optical microscopy maps. Using our results, we propose a new machine learning based criterion for diagnosing a physical system's proximity to criticality.

Dynamical disorder in the lead halide hybrid perovskite $CH_3NH_3PbCl_3$

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Lead halide perovskites are known for their structural instabilities and atomic fluctuations, yet the microscopic mechanisms leading to their exceptional photovoltaic and optoelectronic properties remain to be solved. In the present work, we combine several neutron scattering techniques to reveal the microscopic mechanisms at play in the organic-inorganic perovskite $CH_3NH_3PbCl_3$. We uncover low-lying transverse acoustic phonons at the Brillouin zone boundaries, along with overdamped lattice dynamics all along the Brillouin zone edge in the cubic phase, reminiscent of two-dimensional domains of fluctuating $PbCl_6$ octahedra, along with large displacements of the Cl and methylamonium cations which may play a role in the formation of photo-induced polarons. We use high-resolution spin-echo neutron spectroscopy to investigate the possible coupling between the relaxational dynamics of the off-centered displacements of the halide and A-site cation and the inorganic framework fluctuations. A resolution-limited central peak appears at the X and M Brillouin zone boundaries when cooling down to lower-symmetry phases, bringing evidence for a possible coupling between the lattice dynamics and local polar states.

Effect of hydration on the properties of a superionic conductor $M_2Ti_2O_5.(H_2O)_x$

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The search for new materials containing non-critical mineral resources with remarkable physical properties for numerous applications, for example energy storage, is one of today's major goals.

In addition to the safety aspect, the solid electrolyte which constitutes the supercapacitor, is a crucial element whose main requirement is a high ionic conductivity and a dielectric equivalent permittivity at room temperature. The family of compounds $M_2Ti_2O_5.nH_2O$ (MTO) with M an alkaline element is a solid electrolyte, which presents interesting electrical and electrochemical properties that can be controlled by tuning the hydration rate. For instance, a very promising ionic conductivity of 10^{-3} S/cm and a colossal permittivity of 10^9 have been measured for $Rb_2Ti_2O_5{\cdot}nH_2O$, which are not observed for the dehydrated compound[1].

The mechanism of the transport properties of the ionic species present in these compounds remains unknown to date. Therefore, it is of primary importance to focus on the study of the formation and conduction of the mobile ion(s) and to identify their nature.[1]

In this study, the crystallographic structure and chemical stability of RTO and KTO have been characterized with X-ray diffraction (XRD), TGA and FT-IR [1,2]. Furthermore, new compound containing both potassium and rubidium (RKTO) have been investigated.

At this conference, the hygroscopic character of the compound and the chemical stability will be focused on, by presenting the different results of FT-IR and XRD measurements. Finally, the link between these chemical properties and the ionic conductivity of the compound will be presented.

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Electric-field switching between multiple crystallographic phases in the brownmillerite $Ca_2Al_2O_5$

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Brownmillerites $ABO_{2.5}$ are oxides possessing a crystallographic structure parent from the perovskite structure ABO_3 with an ordered sublattice of oxygen vacancies [1]. The oxides possessing such a structure are thus formed by alternated (001) atomic layer following the sequence $AO|BO_2|AO|BO$, where the planes BO consists in 1D chains of oxygen tetrahedra, while BO_2 planes are the regular planes of octahedra usually found in perovskites. The oxygen tetrahedra can be tilted and their associated chains are chiral. Due to their particular structure, Brownmillerites form a promising family of materials for applications in several domains. The properties of Brownmillerites can indeed be tuned either by controlling the distribution of chains with different handednesses [2,3], or by triggering topotactic transitions, by benefiting from the anisotropic ionic conductivity, higher within the oxygen-vacancy channels [4,5].

We have performed first-principles calculations to study the effect of an external electric field on the stability of different crystallographic phases. We considered the non-magnetic $Ca_2Al_2O_5$ oxide as an example. Because the chirality of the chains of oxygen tetrahedra are linked to the formation of electric dipoles, the configuration of chain handedness determines if the formed phases are polar or not. Considering the polar phase *Ima2*, we found that reversing the direction of the electric polarization necessitates going through different intermediate phases. Even if these phases display close total energies, the barrier to overcome to switch between two phases, i.e. to reverse the electric dipole direction or the handedness of a chain, is quite high. Selecting a particular phase would thus certainly require applying an electric field at high temperature or inducing an additional strain.

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Electronic/ thermal transport and thermoelectric phenomena in implanted diamond nanostructures

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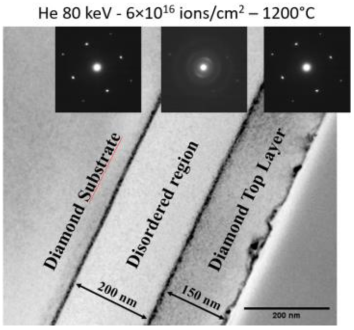
The interaction between phonons and electrons is known to be at the origin of large values of the Seebeck coefficient at low temperatures, a phenomenon known as “phonon drag” in the Seebeck perspective in which a fraction of the phonon momentum, induced by an applied thermal gradient, is transferred to the electron gas. While phonon drag produces high Seebeck values, the thermoelectric community has long ignored it, since it is associated with phonons of long mean free paths and therefore high lattice thermal conductivity. This was the case until 2008 when Boukai et *al*. ***[1]*** confirmed in a study with Silicon nanowires, that it is possible to have a large phonon drag at high temperatures even if the system has low thermal conductivity. In 2015, the group of ZX Chen, at MIT published a paper where they rationalize it with *ab-initio* simulations by considering the coupling between the two Boltzmann equations (electron and phonon transport) through the electron-phonon interaction ***[2]***. They showed that the phonon states that contribute predominantly to heat transport are separated in phase space, in energy, and wave vector from the phonon states that couple to electrons and cause the "phonon drag" effect. In this project, we investigate the thermal and electronic transport properties of conductive channels embedded in crystalline diamond. We aim to separate the phonon gas and the electron gas into two different media and try to have them interact to produce the phonon drag effect. This poster demonstrates how to create a conductive buried region of low thermal conductivity in a matrix of the highest known thermally conductive material in nature and the sample preparation for transport studies with some initial results.



Transmission electron microscopy image of one of our implanted diamond which illustrate the buried channel (disordered carbon) embedded in crystalline diamond.

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Evidence of metal/insulator nanodomains in V_2O_3 mapped by variable-temperature electron spectromicroscopy techniques

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Exploiting abrupt phase transitions in transition metal oxides is a promising approach for the development of advanced information processing and storage systems. V_2O_3 considered as a prototypical system of the metal-to-insulator transitions (MITs) where they can be activated under external stimuli such as temperature (T), pressure, or chemical doping 1] but hardly technologically feasible. Recent demonstrations from electric pulses yield transitions between Mott insulator and strongly-correlated metal in $(V_{1-x}Cr_x)_2O_3$ systems with real potential capabilities for non-volatile memories and neuromorphic applications [2].

However, all these electronic transitions rely on their relationship between structural and electronic degrees of freedom. For instance, when cooled below 160 K, V_2O_3 presents a symmetry breaking (from hexagonal to monoclinic), associated with (i) a magnetic transition to an antiferromagnetic (AFI) ordered state, (ii) a large volume change (+1.4%) and (iii) an IMT yielding a resistivity change of 7 orders of magnitude. This T-driven MIT has been extensively studied at the macroscopic scale [1], and remains still a perfect arena to probe *in situ* the V_2O_3 structural and electronic evolutions at the finest scale. Recently, the microscopic electronic coexistence of insulator/metallic (I/M) domains has been mapped within both $(V_{1-x}Cr_x)_2O_3$ crystals and thin films by *in situ* scanning photoemission spectroscopy [3], PEEM [4] and nano-IR [5] with 25nm spatial resolution at best. In addition, combined micro-XR and nano-IR experiments have highlighted competitive mechanisms between structural and electronic contributions during this temperature-induced MIT [6]. These latest investigations also demonstrates the cautions and possible experimental limitations when it comes to accurately mapping the dynamics of mechanisms within regions of interest of a few tens of nm by combining different instruments, hence the need to perform structural and electronic experiments within the same instrument. Advanced monochromated electron spectromicroscopes emerged this last decade as real game-changers for nanomaterials characterization.

Here we performed *in situ* monochromated STEM/EELS experiments on the NION CHROMATEM 200 MC with variable-T options under cryo-conditions to vary continuously the temperature conditions across the IMTs. For each probed temperature, we associated mapping of relevant spectroscopic electronic excitations (from IR to soft X-ray) with an ultra-high EELS resolution at the nm scale and the local structural features (symmetry and lattice parameters) determined by 4D STEM nano- and microdiffraction.

The T-activated V_2O_3 transition was investigated in V_2O_3 single crystals to give a direct, and local access to the structural and electronic evolution. During low-T thermal cycling through the resistive transition, EELS spectra acquired in the low-loss regime present a characteristic signature at 1.1eV only in the metallic phase. Upon cooling, the abrupt MIT was monitored while the coexistence of I/M nanodomains was evidenced upon heating over few degrees yielding the propagation of the electronic domain wall. Remarkably, periodic contrast HAADF inhomogeneities appeared solely in the insulating state. 4DSTEM nanodiffraction experiments reveal the local distribution of monoclinic/rhombohedral phases coexisting in the insulating domains. The observation of the insulating hexagonal phase at low-T suggests the presence an analogous paramagnetic insulating (PI) phase of large volume, as confirmed by the jumps in lattice parameters observed at the transition. This PI-like phases emerge also at the I/M domain wall, as a precursor of the metallic phase.

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Facing the challenges of superconducting infinite-layer praseodymium nickelate synthesis

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We present preliminary results of ongoing research to obtain superconducting thin films of the hole-doped infinite-layer praseodymium nickelate phase onto $SrTiO_3$ and LSAT substrates. A major challenge concerning the synthesis of superconducting nickelate films is the growth of high-quality epitaxial films of the parent perovskite phase, $Sr_{0.2}Pr_{0.8}NiO_3$, free from disorder and extended defects. We have synthesised $Sr_{0.2}Pr_{0.8}NiO_3$ films up to $\approx$ 10 nm in thickness by Pulsed Laser Deposition, where layer-by-layer growth is evidenced on both systems by Reflection High-Energy Electron Diffraction (RHEED) oscillations, and characterised their structural and electrical transport properties. Hall effect measurements on both substrates show similar trends. The perovskite films were reduced via oxygen deintercalation through topotactic reduction using CaH_2. Upon reducing annealings, we observed diffraction peaks in the symmetric θ-2θ scans consistent with the infinite layer phase, exhibiting incomplete superconducting transitions without reaching a zero resistance state. Furthermore, the sample-to-sample variations observed in films grown and reduced under identical conditions present additional challenges. Further understanding is required to clarify the role of epitaxial strain induced by the substrate on the optimal conditions for the topotactic transformation of the parent perovskite $Sr_{0.2}Pr_{0.8}NiO_3$ leading to the reduced superconducting phase.

Ferroelectric two-dimensional electron gases based on $SrTiO_3$ thin films

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Abstract

Two-dimensional electron gases (2DEG) at $SrTiO_3$ (STO)-based oxide interfaces gained a wide interest not only from the fundamental aspect but for their potential usage in technological applications.[1-2] A rich variety of emergent phenomena such as quantum Hall effect, Shubnikov-de Haas oscillations, Rashba effect, 2D superconductivity, inverse Edelstein effect etc. were observed at such interfaces.[3-4] For future integration, it would be more interesting to create the high mobility 2DEG in STO thin films rather than using the single crystal substrates. In addition, introducing epitaxial strain in thin films could be used to manipulate the properties of STO and therefore of the 2DEG based in STO thin films. However, to date reports on interfacial 2DEGs based on STO films have shown mixed results, with mobilities only in the range of 10 cm^2/Vs at low temperature vs more than 1000 cm^2/Vs for 2DEGs based on single crystal STO.[5-6]

In this presentation, we will present results on STO 2DEGs based on STO films grown by hybrid oxide molecular beam epitaxy and formed by a redox process through the deposition of ultrathin Al films by sputtering. The mobility is more than one order of magnitude higher than in previous reports. We can then utilize epitaxial strain to introduce ferroelectricity (FE) in such films and hence, in 2DEGs created at their surfaces. We will show our data on strained STO thin films epitaxially grown on LSAT substrate in which Raman study shows the signature of FE. The transport data of 2DEG in STO thin films also shows the coupling between FE and electronic properties.

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Heavy fermion behavior in self-intercalated VS_2 dichalcogenide

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MX_2 layered transition metal dichalcogenides exhibit a large variety of interesting physical properties including charge density waves, superconductivity, or topological phases [1]. Some of them are serious candidates for applications in electronics as transistors and in optics as emitters and detectors. In a bulk form, the common way to tune their properties is the cationic intercalation in the van der Waals gap, with an effective charge transfer to the electronically active MX_2 layer that can modify the electronic band structure.

Here we present the case of (self-)intercalated V_xVS_2 with a strong interaction between intercalating and intercalated V cations. We focus on $V_{1/4}VS_2$ (or V_5S_8) and $V_{1/2}VS_2$ (or V_3S_4) with the so-called NiAs-defect structure, for which we have determined the magnetic susceptibility, specific heat, and resistivity at ambient and high pressure. We show that these compounds develop relatively strong electronic correlations when compared to other transition metal sulfides, which is in accordance with a high density of states at the Fermi level. Furthermore, their resistivity also exhibits non-Fermi liquid behavior, at high pressure for V_5S_8 and at ambient pressure for V_3S_4. We will discuss the crossover from the Fermi to non-Fermi liquid phase in terms of Kondo physics and RKKY interactions.

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Improper Ferroelectricity Induced by Oxygen Rotation in Magnetic Doubly Ordered Perovskite

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Magneto-electric multiferroics are defined as a class of materials combining ferroelectric and ferromagnetic properties in a single phase. They are drawing considerable research interests not only for the variety of attractive fundamental phenomena but also for potential technological applications.

Recently, a new approach was proposed to induce a spontaneous ferroelectric polarization by a combination of two nonpolar rotation modes of the oxygen octahedra in magnetic materials, the so-called "Hybrid Improper Ferroelectricity (HIF)". Furthermore, the HIF mechanism has the potential to enable magnetoelectric coupling in layered perovskites. On the basis of the thought above, we have turned our attention to a class of doubly ordered perovskite compounds AA'BB'O6. In their structures, the cations on the B-sites order in a rock-salt type, which is fairly common and has been observed in many A2BB'O6 compounds. The layered ordering of A-sites, which is rather rare, is found simultaneously in this sort of compound. The uncommon ordering on the A-sites is stabilized by the second-order Jahn−Teller (SOJT) distortions of the highly charged B' cations.

The compounds of the doubly ordered perovskite family NaLnTWO6 (Ln = Lantanides, T= transition metal) were synthesized by solid-state reaction, some of them been prepared under high-temperature and high-pressure conditions. Their structural properties were investigated by synchrotron X-ray powder diffraction and neutron powder diffraction. Most of them have the polar space group $P2_1$ symmetry, as confirmed by second harmonic generation measurements. The decomposition in terms of symmetry modes demonstrate that the polar mode is induced by two nonpolar modes in a manner of Hybrid Improper Ferroelectricity [1,2].

We investigate their magnetic properties by magnetization [3] and neutron diffraction measurements. All of them show long range magnetic ordering, more or less complex depending on the nature of the rare earth. Their electrical properties are complex, showing magneto-dielectric properties for some Ln and T. They will be discussed in this poster.

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$LaFeSiO_{1-\delta}$: a novel superconducting member of the Fe silicides family with squeezed FeSi layers

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Since their discovery in 2008, iron-based superconducting pnictides (As, P…) and chalocgenides (Te,Se…) are now a well-established class of unconventional superconductors, spanning multiple structural families, with T_c up to 55 K in bulk materials [1]. This category of superconductors has recently been extended to other layered materials where pnictogen/chalcogen atoms are replaced by crystallogen elements: either with Ge in YFe_2Ge_2 (T_c ~ 2 K) [2] or Si in LaFeSiH (T_c ~ 10 K) [3].

In this work, we present the discovery of a new compound obtained by oxygenation of LaFeSi [4]. The resulting unexpected crystallogenide, $LaFeSiO_{1-\delta}$, showed very interesting properties. Our detailed study based on complementary experimental probes reveals that this crystallogenide is superconducting with a relatively high T_c ~ 10 K, regarding its strongly squeezed Fe-Si anion height, below 1 Å, challenging the usual relationship between structure and superconductivity in Fe-based compounds (Fig.1.).

Its unique crystal structure has a strong impact on its electronic properties. Just above T_c, its resistivity shows a non-Fermi liquid behavior, a signature of its electronic correlations. This correlated behavior is also visible in the NMR data which evidences weak antiferromagnetic fluctuations. The calculated electronic structure of LaFeSiO is significantly changed compared to the one of the canonical LaFeAsO pnictide. Its Fe-related Fermi surface, consisting almost uniquely of hole pockets, suggests another kind of electronic correlations and then a different related superconducting mechanism than the usual the s±-mechanism. Finally, the location of $LaFeSiO_{1-\delta}$, LaFeSiH and $LaFeSiF_x$ [5] superconductors in the phase diagram points towards the existence of a new emerging superconducting dome related to Fe-silicides.

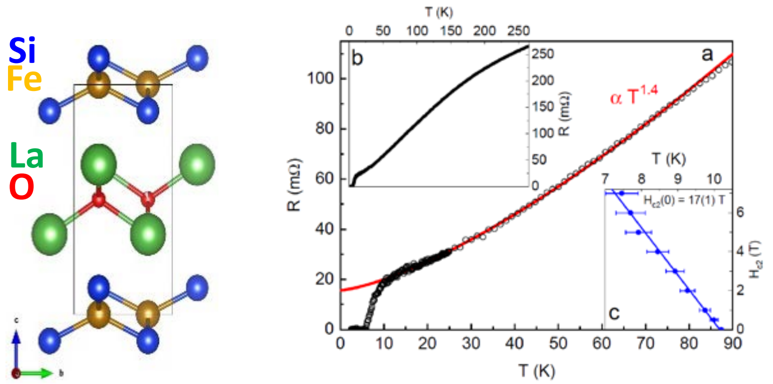

Fig. 1: ***Left:*** *crystal structure of* $LaFeSiO_{1-\delta}$. ***Right:*** *resistivity measurement of* $LaFeSiO_{1-\delta}$ *(full temperature range dependence in left inset and related* H_{c2} *critical field as a function of temperature in right inset).*

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Magnetic frustration revealed by Inelastic Neutrons Scattering in $BaFe_2Se_3$

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Magnetoelectric multiferroicity is a property of solid state that arise from coupling ferroelectricity to magnetic order. This unique property offers multiple potential applications but its microscopic origin is a fundamental challenge. In most of cases, it appears in systems presenting complex magnetic order, a complexity usually coming from an underlying magnetic frustration. Two mechanisms are often proposed for such coupling : the exchange striction and the Dzyaloshinskii Moriya interaction.

Recently, it has been shown that the quasi-1D Fe spin ladder $BaFe_2Se_3$ exhibits multiferroicity [4]. The magnetic order takes the form of staggered ferromagnetic blocs along the ladder. All spins being colinear, the Dzyaloshinskii-Moriya mechanism is thus excluded. In addition, a set of non frustrated magnetic exchange interactions has been proposed from inelastic neutron scattering measurement on powder [1], ruling out the exchange striction mechanism.

We present here our INS results performed on single crystal of $BaFe_2Se_3$ and Time-of-Flight spectrometer. In addition to directional information of the dispersion, we observed additional modes not reported on the powder experiment. Thanks to spin wave calculations [3] and Monte Carlo simulations, we determined a different set of exchange parameters that better describes the spin dynamics. This new information not only offers a better interpretation for the multiferroicity in this system, but also provide new perspective to understand other properties of this system and other members of the family [5].

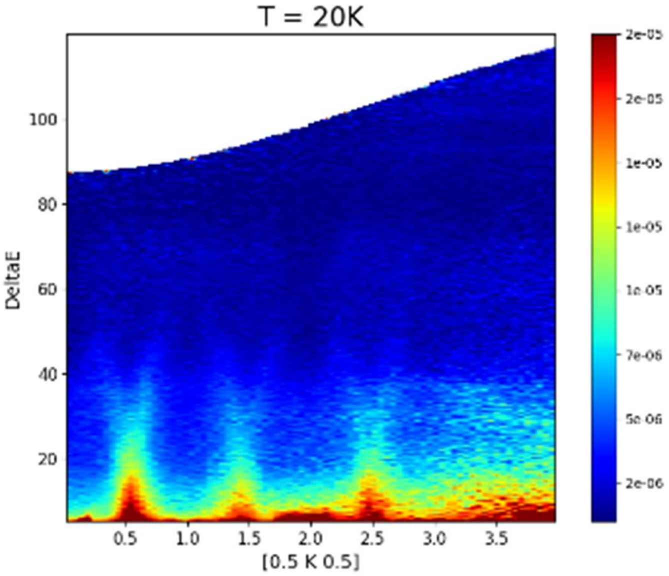

Figure 1: Inelastic neutron scaterring map of $BaFe_2Se_3$ along [½ k ½] direction.

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Nanoscale control of oxygen vacancy distribution in transition metal oxides by E-AFM

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The Nickelate family is characterized by the chemical formula $RNiO_3$ where R is a trivalent rare-earth element, and is fascinating thanks to its wide range of physical and structural properties. One of the main interests on this family is the possibility to get superconductivity due to their similarity with the cuprates: Nickel and Copper are isoelectronic with the oxidation states Ni^{+1} and Cu^{+2}. Thus, the quest of superconductivity in nickelates has attracted a lot of attention in the last decades until 2019, when Hwang et al.[3] synthesized for the first time an infinite-layer nickel compound and observed superconductivity at very low temperature (T_c~9-15 K) in $Nd_{0.8}Sr_{0.2}NiO_3$ and in $Pr_{0.82}Sr_{0.18}NiO_2$ compounds [3,4,5]. However, the technique used to obtain the infinite-layer is hardly reproducible: starting from obtaining the correct perovskite phase, which requires high temperature and controlled oxygen pressure to stabilize the Ni^{3+} oxidation state, and following by the complexity in the subsequent chemical reduction with CaH_2. Many parameters of such chemical topotactic reduction (e.g. tube size, temperature and annealing time or amount of CaH_2) are difficult to recreate among research groups and only three of them (none in Europe) had successfully managed in obtaining the superconducting infinite-layer phase of nickelates. Still, this type of topotactic transformation cannot provide spatial resolution of the transformation, which limits its application in many technologies.

In this work, we propose an alternative and more easily accessible technique to manipulate the oxygen content in nickelates with the aim of obtaining the superconducting infinite-layer phase. For that, we will use the electric field produced by an atomic force microscope (AFM) tip under specific conditions. This new approach will provide us with micro-metric control of the chemical transformation and therefore, on the superconductivity compared to the usual topotactic transformation. Similar approach was already used by Ferreiro et al.[6], who achieved a reversible transformation between $SrFeO_3$ and $SrFeO_{2.5}$ structure or by Lucia et al.[7], who manipulated the oxygen vacancies in $SrTiO_3$ thin films by applying a current to the AFM tip. Here, we will show the first steps towards the manipulation of oxygen vacancies in our few nanometers thick $Pr_{0.80}Sr_{0.20}NiO_3$ thin films grown on LSAT substrates to obtain the infinite-layer phase. Different techniques such as Raman spectroscopy or Kelvin Probe Force Microscopy (KPFM) will be used to assist us in determining the possible structural change. In the event of success, the micrometric-control on the formation of the superconducting phase in nickelates would directly lead to the possibility of designing novel superconducting devices or architectures drawn with the AFM tip, opening a vast field of applications.

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Neutron diffraction in $MnSb_2O_6$: Coupled chiralities in a polar magnet

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Multiferroic materials have been intensively studied these last decades for their interesting physics and their promising magnetoelectric applications [1]. Magnetoelectric coupling is particularly strong when a non-centrosymmetric magnetic ordering, such as spin spiral, is breaking the inversion symmetry, inducing a spontaneous electric polarization. Materials having a crystallographic chirality are further interesting in the sense that their structure couples to magnetism. This is the case of $MnSb_2O_6$ which crystallizes in $P321$ space-group. Similarly to iron based langasite ($Ba_3NbFe_3Si_2O_{14}$[2]), the building block in terms of magnetic interactions is the isolated MnO_6 octahedra resulting in chiral super-super-exchange pathways (Mn-O-O-Mn) along the c-axis. The Mn atoms form a triangle in the unit cell, where the magnetic moments in the (ab)-plane are dephased by 120° and follow a cycloidal modulation along the c-axis [3], in contrast to an helical modulation in iron langasite. In analogy to the latter compound, the sense of rotation of the spins within the Mn triangle or along the propagation vector define magnetic chiralities, which are directly linked to the structural chirality through Heisenberg interactions. Due to the presence of threefold magnetic domains below $T_N = 12$ K, this compound was predicted to have an unique switching mechanism, which was explained by an ambiguous magnetic ground state [4]. By a combination of unpolarized and polarized neutron diffraction techniques, we have extensively studied both the nuclear and magnetic structure of $MnSb_2O_6$ [5]. A mixture of chiral structural and magnetic domains was found in our single crystal. We subsequently propose a mechanism leading to electric polarization based on coupled structural and magnetic chiralities.

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Nuclear and magnetic structure of manganite epitaxial thin films

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The field of antiferromagnetic spintronics has been the object of active research over the past decade for the next generation of spin-based devices [1,2]. A particular focus has been on the design of new materials, specifically thin film preparation and detailed understanding of their magnetic properties.

Doped manganite films have shown interesting functional properties suitable for such devices [3]. However, obtaining exact knowledge of film crystallography is still a challenge and diffraction methods are good candidates for such studies. The neutron diffraction (ND) instrument, D10 at ILL has been increasingly used for measurements on such films [4,5] as well as X-ray diffractometer at SmartLab (CEA-CNRS, Grenoble).

In this framework, we use ND and X-ray diffraction to solve nuclear and magnetic structure of epitaxial thin films. We are interested in $La_{2/3}Sr_{1/3}MnO_3$ (LSMO) thin films deposited on Si substrate with a $SrTiO_3$ (STO) buffer layer. We have employed SQUID magnetometer, electron diffraction and microscopy to complement the diffraction data. Our results show that these films can be treated as single crystals to measure diffraction peaks and determine the nature of magnetic spin configuration in the system.

In this talk, I will present our most recent results obtained on these manganese oxide thin films.

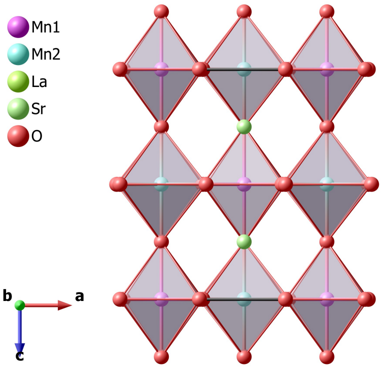

Figure: Schematic of the LSMO film structure deposited with STO buffer layer on Si substrate

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Prospection of chalcogenide thermoelectric materials assisted by active learning and Bayesian optimization

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Chalcogenide materials like Bi_2Te_3 or GeTe are well-known for their good thermoelectric properties either at room or high temperatures. Numerous compounds with further improved thermoelectric properties remain to be discovered for supporting a multi-modal approach to a sustainable energy future. To this end, the rational design of thermoelectric materials can be drastically accelerated thanks to artificial intelligence techniques by comparison to the classic and time-consuming trial-and-error methodology. In this sense, efficient and insightful studies assisted by machine learning can be conducted by encompassing experimental processes and expert knowledge. In this framework, we investigate new chemical compositions of substituted GeTe supported by machine learning. Traditional as well as cutting-edge deep learning techniques have been considered along with Bayesian optimization for proposing candidates with improved performance. Moreover, this opens the possibility to bring novel insights into the underlying physical mechanisms in these very interesting metavalent materials. Here we will present the preliminary results of this work.

Quantum fragmented states in pyrochlores oxides

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Since the 2000s, the discovery of spin ices in rare earth oxides of pyrochlore structure has aroused great interest. This is indeed a new state of matter, lacking long-range magnetic order, but where the Ising spins, which occupy the vertices of the tetrahedra that form the pyrochlore structure, arrange themselves according to a local organization rule, which stipulates that each tetrahedron must have 2 incoming and 2 outgoing spins. This results in a macroscopically degenerate state, associated with a non-zero entropy at zero temperature. An elegant way to describe this state is to consider the Ising spins as the lines of an emerging field, along with a gauge charge defined as the sum of the 4 spins of a tetrahedron. In this "electodynamic" description, the spin ice is then a state of zero divergence (or zero charge). More recently, the notion of fragmentation has been proposed, to describe new states of matter, where the charge is not zero and ordered, but where the spins remain disordered [1,2]. This is what happens, for example, in a moderate magnetic field applied along the [111] direction of spin ices, or in certain compounds as $Ho_2Ir_2O_7$ or $Dy_2Ir_2O_7$ [3,4]. In this presentation, we are particularly interested, thanks to MC calculations, in the fate of these fragmented states when the spins are no longer of Ising nature, but where the transverse spin components are coupled by additional "quantum" terms. This approach allows to describe "quantum" fragmented states. We observe in particular that such states occupy a large area of the phase diagram. Moreover, under certain conditions, new fragmented states can even appear due to these additional couplings. These results are put in perspective with recent experimental observations.

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Quantum oxide two-dimensional electron gas with imprinted ferromagnetism for spin-charge interconversion

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A known property of 2DEGs at the interface of materials where inversion symmetry is broken, is the Rashba spin-orbit coupling [1], which endows the electronic bands with unique spin textures and couples the spin of mobile electrons to their momentum. In a 2DEG with Rashba coupling, an external electric field can induce a large-scale spin polarization and provide efficient spin-charge interconversion via the direct or the inverse Edelstein effect (EE/IEE) [2,3]. In this work, we studied theoretically the two-dimensional electron gas (2DEG) at the interface between strontium titanate ($SrTiO_3$) and a ferromagnet. By introducing ferromagnetism as an additional degree of freedom, we hope to uncover a range of new physical phenomena. We use an 8-band tight-binding Hamiltonian to model the t_{2g} bands relevant for the formation of the 2DEG [4] at the STO surface and added a Zeeman-like term, to account for the exchange field of the ferromagnet.

Within the semiclassical Boltzmann approach, we can simulate the charge-spin interconversion efficiency [5]. We found that the EE's ability to convert charge to spin could be enhanced by the out-of-plane exchange field. Our examination of the band structure and spin textures gave us insight into the relationship between Rashba spin-orbit coupling and ferromagnetism.

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Reversible superconductivity suppression under light ilumination in exfoliated $Bi_2Sr_2CaCu_2O_{8+x}$

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Persistent photoconductivity and photoinduced superconductivity can be found in $YBa_2Cu_3O_{6+x}$, causing the critical temperature and conductivity of this material to increase upon light illumination. These changes have been related with changes in the carrier mobility and the presence of CuO chains in this material. Nevertheless, $Bi_2Sr_2CaCu_2O_{8+x}$ does not present these CuO chains, blocking these photoinduced effects. Several works in BSCCO thin films have demonstrated that, in fact, there is a decrease in conductivity and critical temperature of up to 3K upon illumination, but without reversibility. In our experiment we have exfoliated BSCCO on top of Si/SiO_2 substrates and have illuminated them with visible monochromatic light. Surprisingly, a reversible transition between a superconducting and a metallic state appears upon illumination at 100K. These results open new questions about the possible origin of photoinduced effects in this material.

Spectro-microscopic investigation of 2DEGs in $KTaO_3$ interfaces

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The 2DEGs in the 5d perovskite $KTaO_3$ (KTO) interfaces exhibits intriguing properties such as superconductivity [1-3], spin-charge interconversion which can have direct applications in spin-orbitronics [4], etc. Here we study the Aluminium deposited-$KTaO_3$ substrates with a focus on the emergence of 2DEG and how it influences the physical properties of interest in these. A microstructural and spectroscopic understanding of these interfaces is much appreciated in this direction. With this motivation, we conduct a study involving Scanning Transmission Electron Microscopy (STEM), Electron Energy Loss Spectroscopy (EELS) (Done at STEM Lab in LPS Orsay) and Standing Wave - Hard X-ray Photoemission Spectroscopy (SW-HAXPES) (Done at GALAXIES Beamline in Synchrotron SOLEIL). STEM-EELS provides insights into the changes in the local chemistry and electronic structure together with an atomic scale resolution. On the other hand, SW-HAXPES is a depth selective and non-destructive technique, with a strong sensitivity to chemical differences in each layer. This combination enables us to extract the photoemission spectra from the interface separately. Such a combined study with STEM-EELS on the differences in a microscopic level and HAXPES on a macroscopic level unfolds the more interesting physics in these systems.

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Superconducting memristors based on metal/cuprate tunnel junctions

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Memristors are a family of resistive switching devices with promising properties such as a continuum of non-volatile resistance states (instead of the conventional two in standard binary memories) driven by the history of applied voltages. Within this framework, we propose a new class of superconducting memristors based on cuprate oxides with high critical temperature T_C, which will allow bringing memory effects to the realm of superconducting electronics. Those memristors consist of tunnel junctions between $YBa_2Cu_3O_{7-\delta}$ (YBCO), which is the archetypal high-temperature superconductor with T_c~90K, and high reduction potential, and different metals with low reduction potentials, namely Al, W, and Co. In this type of device a non-volatile, reversible resistive switching is created via a redox reaction between the oxide superconductor and the metallic electrode, which modifies the interfacial properties and creates a tunable tunneling barrier[1,2]. This redox reaction can be triggered and controlled via two external stimuli: electrical field and visible light. Here we focus on the characterization and optimization of the device properties. Depending on the metal used as the electrode and its size, we can obtain a reversible and non-volatile switching of the conductance within a continuum of states which are much as two orders of magnitude afar (from 10^{-3} S to 10^{-5} S). These properties make these superconducting memristor devices promising for neuromorphic applications.

Work supporter by ERC POC “SUPERMEM”

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Superconductivity and Rashba spin orbit coupling in $KTaO_3$ (111) microdevices

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The recent discovery of superconductivity in two dimensional electron gases (2DEGs) based on quantum paraelectric $KTaO_3$ (*1*) has revived efforts to explore emergent physics at oxide interfaces, in line with the works on $SrTiO_3$-based 2DEGs (*2*). With a combination of Rashba spin-orbit coupling, magnetism and 2D superconductivity, such systems have the potential to be a platform for the development of topological quantum electronics (*3*). However, the fabrication of devices with $KTaO_3$ interfaces proves challenging. High temperature processing steps exclude simple UV lithography and ion beam etching during which adventitious oxygen vacancy doping shorts the 2DEG, which is also damaged in oxygen-rich atmosphere. Thus, the large majority of studies on superconducting $KTaO_3$-based 2DEGs involve unpatterned samples (*4*).

Here we present three successful routes to fabricate superconducting AlO_x/ $KTaO_3$ (111)-based microdevices and demonstrate the ability to finely tune the carrier density and the superconducting critical temperature by field effect (*5*). We also present our first results of Rashba coupling measurements by bilinear magnetoresistance. The methods could be extended to the patterning of nanoscale devices and help to investigate the properties and origin of the superconducting phase at these interfaces.

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Superionic conductors with virtual cathode creation

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The search for new materials containing non critical mineral resources with remarkable physical properties for numerous applications, for example energy storage, is one of today's major goals.

In the past years, the ternary titanium oxides from the $M_2Ti_nO_{2n+1}$ (MTO) family, where M is an alkaline element, have attracted a renewed interest owing to their unique physical and chemical properties [1][2][3].

As a matter of fact, previous studies have revealed a remarkable colossal equivalent dielectric permittivity ($\epsilon_{RTO} = 10^9$ and $\epsilon_{KTO} = 10^7$) and a high ionic conductivity (σ_{RTO} =0.1mS.cm^{-1} and σ_{KTO} =0.01mS.cm^{-1}) at room temperature, for hydrated $Rb_2Ti_2O_5$ (RTO) and $K_2Ti_2O_5$ (KTO) [3][1]. These promising properties make RTO and KTO good candidates for a solid electrolyte working at room temperature. In addition, the discovery of RTO's memristive effects driven by ionic diffusion or migration have been investigated.

For this research project, the synthesis of RTO and KTO single crystals and ceramics has been developed and their crystallographic structure characterized with X-ray diffraction (XRD). In order to investigate the charge distribution inside the samples, an experimental technique called the Pressure-Wave-Propagation (PWP) experiment has been performed on single crystals and ceramics with different types of electrodes, showing the same charge dynamic response. These materials demonstrate an accumulation of negative charges near the anode and an absence of charge at the cathode, indicating a virtual cathode that shifts inside the materials, regardless of the type of electrode [2].

At last, these findings are a first step to relate the macroscopic behavior (colossal dielectric permittivity) to the the microscopic mechanisms. This will lead to a deeper understanding of the observed phenomena.

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Theoretical modelling of superconducting nickelates

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Recent discovery of superconductivity in **Sr** doped infinite layered nickelate $\mathbf{Nd}_{1-x}\mathbf{Sr}_x\mathbf{NiO}_2$ opens up the need to revisit the electronic structure and physical properties of nickelates. In experimental synthesis of layered nickelates from **Ni**-based rare earth perovskite, critical aspects such as stoichiometric instability accompanied with electronic and magnetic phase change, play an important role. Moreover, plethora of many conventional and unconventional phenomena are found in these Quasi-2D (Crossover between 2D and 3D) systems which can be understood on reconsidering similarities and difference between nickelates and cuprates. In both cases superconductivity is achieved by doping a parent compound. Doping is realized by atomic substitution of rare-earth (**Nd** substitution), resulting emergence of new effects from disorder and electronic correlations from the rare-earth.

Based on this aspect, a complementary theoretical approach , preliminarily using a Tight Binding (**TB**) model, is attempted with aim to modify and generalize the Dynamical Mean Field Theory (**DMFT**).The model parameters are first chosen phenomenologically to ensure the bench marking of the previous available results.

Thermal conductivity in the 1D spin ½ cuprate SrCuO2

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$SrCuO_2$ is a 1D magnetic compound that exhibits a remarkably large and anisotropic thermal conductivity. Measurements have shown that its ability to transport heat along spin chains is close to 800 $W.m^{-1}.K^{-1}$, comparable to that of Copper [1]. While phonons are the main heat carriers in insulators, spinons, unconventional magnetic excitations typical of 1D magnets, strikingly participate to these very peculiar thermal properties in $SrCuO_2$ [2]. Understanding these thermal properties may unravel new aspects of the ground states of such spin ½ chains [2]. The aim of this work was to estimate the contribution of the spinons to the thermal conductivity $\kappa(T)$ of $SrCuO_2$ using a different method than the one described in [1]. Two types of quasiparticles have to be considered to characterize heat transport $\kappa(T)$ in this compound, phonons and spinons, with $\kappa(T) = \kappa_{Ph}(T) + \kappa_S(T)$. First, we focused on the estimation of heat transport by phonons, $\kappa_{Phonons}(T)$ [3]. Theoretical calculations based on DFT force constants were performed initially to obtain the phonon dispersion in $SrCuO_2$, which was subsequently compared with inelastic neutron scattering measurements. Our calculations were found to be in good agreement with experimental data, thus validating the approach. From the phonon dispersion spectra, we then computed $\kappa_{Phonons}(T)$. Strikingly, it was found to be very anisotropic, being much larger in the $\vec{c}$ direction parallel to the spin chains. By subtracting the calculated $\kappa_{Phonons}(T)$ to the experimental $\kappa(T)$ along $\vec{c}$, we were then able to estimate the contribution of spinons to the thermal conductivity along $\vec{c}$, $\kappa_{Spinons}(T)$. Our results suggest that the spinons mean free path is much shorter than the phonons' at low temperature , and drops sharply above 40 K, down to a few dozen ångströms only.

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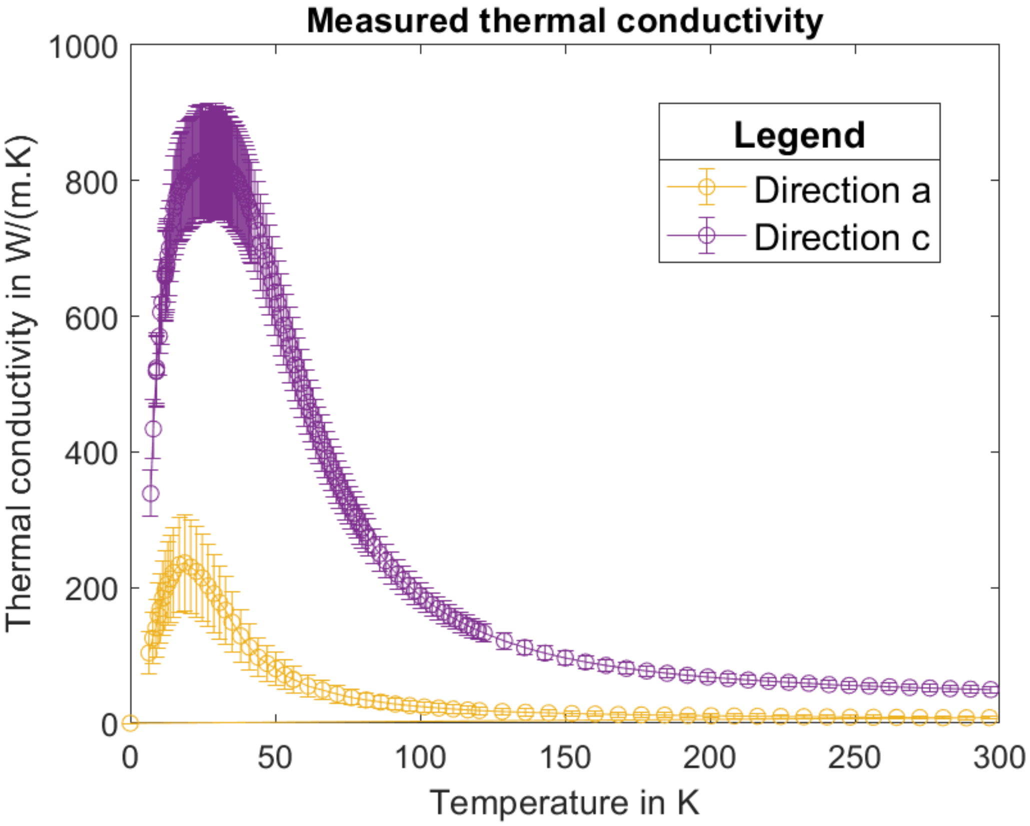

Understanding the insulating-to-metal switching in spinel Ferrites

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Due to the increasing demand for energy and resources in current technologies, searching for energy-efficient, environmentally-friendly and sustainable materials is a today's priority. Spinel ferrites MFe_2O_4 or γ-Fe_2O_3 could be good candidates due to their multifunctionality, cost-effectiveness, and ease to recycle. Some of these oxides are already used and studied for various spintronic applications[1-4] thanks to their ferrimagnetic properties, with high saturation magnetizations and Curie temperatures well above room temperature. In addition, they are also considered for other applications such as energy storage devices, catalysis, sensors, actuators. Understanding the role of defects in this material is very important to assess and improve their performances. Point defects such as vacancies could in particular play an important role in resistive switching mechanisms.[5]

We performed *ab initio* calculations to investigate the effects of cation and oxygen vacancies on the electronic and magnetic properties of an inverse spinel ferrite, considering the insulating $NiFe_2O_4$ as an example. We will discuss which vacancies are expected to form as a function of the experimental growth conditions. We will then explain the electronic-structure and magnetic-properties changes induced by the presence of these defects. Interestingly, we predict that $NiFe_2O_4$ crystals with an excess of Ni cations could display a strongly-spin-polarized hole conductivity.

Keywords: Spinel ferrites, atomic vacancies, Functional oxides

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ZETA$^+$ or how to measure the lifetime of an excitation

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An exemple of a central issue in the development of modern nanotechnologies is the engineering of thermal conductivity of semiconductor materials. Thermal energy is mainly carried here by atomic vibrations, described by quasi-particles called phonons. During its lifetime, a phonon transports a quantum of heat, given by the product of its energy and its speed. Knowledge of the individual properties of phonons is therefore fundamental for applications such as waste heat recovery by thermoelectric (TE) conversion, where one of the main challenges is to identify semiconductor materials with low thermal conductivity. Although the phonon energies and speeds can be measured and calculated easily, access to phonon lifetime is extremely challenging as it requires determination of anharmonicity and detailed disorder modelling. This exemple is not the only one and access to the lifetime of an excitation is a key to improving many materials. A typical inelastic neutrons scattering (INS) experiment of phonons scattering can determine lifetimes up to $\tau \simeq 5$ ps (corresponding to a full width at half maximum of $\Gamma_{FWHM} \simeq 250$ μeV), giving a mean free path (MFP) of the order of 10 nm for a phonon group velocity of 2000 ms^{-1}. As a result, phonon lifetimes have only been accurately measured in a few cases where they are already very short. In order to measure much longer lifetimes, a new method, combining the neutron spin-echo (NSE) technique and three-axis spectrometry (TAS), has been developed : the neutron resonant spin echo (NRSE). NSE, proposed by F. Mezei[1], makes it possible to measure the widths of the non-dispersive excitations in the solids with a resolution of a few μeV, thus improving the typical TAS resolution by about two orders of magnitude. Due to instrumental limitations, this technique cannot be applied to dispersive modes. These limitations were eliminated with the development of the neutron resonance spin echo (NRSE) technique introduced by R. Golub and R. Gähler[2]. According to this technique, two radio-frequency (RF) neutron flippers are installed in a zero magnetic field and replace the long solenoid used in NSE. We are going to present the last improvements of this technique with the upgrade ZETA$^+$ on the TAS IN22.

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