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Jean-Noël Fuchs (Sorbonne Université, Paris)
Carlos Mejuto Zaera (Université Toulouse III)
Vinh Ta-Phuoc (Université de Tours)
Filippo Vicentini (Ecole Polytechnique, Paris)
Matthias Wüttig (RWTH, Aachen)

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Réunion plénière du GDR MEETICC 2025

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Understanding unconventional Solids: Lessons to learn from three Oracles

Matthias Wuttig

RWTH Aachen University of Technology, Germany

Scientists and practitioners have long dreamt of designing materials with novel properties. Yet, a hundred years after quantum mechanics lay the foundations for a systematic description of the properties of solids, it is still not possible to predict the best material in applications such as photovoltaics, superconductivity or thermoelectric energy conversion. This is a sign of the complexity of the problem, which is often exacerbated by the need to optimize conflicting material properties. Hence, one can ponder if design routes for materials can be devised.

In recent years, the focus of our work has been on designing advanced functional materials based on semiconducting chalcogenides with attractive opto-electronic properties, including phase change materials, thermoelectrics, photonic switches and materials for photovoltaics. Many of these materials possess a rather unconventional portfolio of properties. To understand those, one can try to establish close links bet-ween material properties and chemical bonding. However, until recently it was quite difficult to adequately quantify chemical bonds. Some developments in the last decades, such as the quantum theory of atoms in molecules have provided the necessary tools to describe bonds in solids quantitatively. Using these tools, it has been possible to devise a map which separates different bonding mechanisms [1].

This map can now be employed to correlate chemical bonding with material properties. Machine learning and property classification demonstrate the potential of this approach. These insights are subsequently employed to design phase change as well as thermoelectric materials. Yet, it is still highly desirable to identify experimental evidence for unusual chemical bonds that give rise to these properties. To this end, we have devised three 'oracles', i.e., measurement schemes which identify uncon-ventional solids. These oracles classify the response function of solids with respect to bond rupture (studied by atom probe tomography), the excitation of coherent phonons and the infrared reflectivity. The discoveries presented here also force us to revisit the concept of chemical bonds and bring back a history of vivid scientific disputes about 'the nature of the chemical bond'.

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Flatbands from Quantum Scattering on a Honeycomb Network

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Flat bands are one of the central topics across periodic platforms — from Moiré to photonic and mechanical lattices — yet most analyses rely on tight-binding models. In this talk, I will present a complementary scattering approach for quantum wire networks, showing that the honeycomb network generically hosts exact flat bands without fine-tuning. The effect arises from lattice connectivity and symmetry of the honeycomb lattice, which enforce interference among amplitudes on the bonds. I then generalize the result: the flat band persists in honeycomb networks with multiple propagation channels per bond and with symmetry-respecting bond disorder — both necessary for experimental relevance. I will also discuss how weak randomness introduces dispersion, contrast with square and triangular networks with no generic flat bands, and note a 3D diamond analogue with degenerate flat bands. This study provides a practical criterion and diagnostics for mesoscopic, microwave, and photonic implementations, and paves the way for understanding interactions in flat band systems.

Thermodynamic theory of local orbital magnetization

Sariah Al Saati[1], Karyn LeHur[1], Frédéric Piéchon2

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Orbital magnetization is a bulk thermodynamic property which characterizes the existence of electronic charge loops current at equilibrium, in metals and insulators. In a gap of a Chern insulator, the orbital magnetization varies linearly with the chemical potential with a slope equal to the quantized anomalous Hall conductivity plateau.

The modern theory of orbital magnetization for Bloch electrons in multiband systems emerges in 2005. Few years later, Bianco and Resta further derived a heuristic formula for the local orbital magnetization infinite-size systems. Importantly, in order to describe the topological features on a local scale these authors have shown the necessity to introduce an effective local Chern marker.

In the present work we use a thermodynamic perturbative approach to develop a microscopic theory of local orbital magnetization. For Bloch electrons in multi-band systems, we find that the orbital magnetization per sublattice involves quantum geometric quantities that goes beyond the Berry curvature contribution already appearing in the modern theory. We show that these novel features lead to unexpected behavior of the sublattice orbital magnetization in a trivial band gap. For finite-size systems, we derive a novel formula for the local on-site orbital magnetization. This formula provides an alternative expression for the local topological marker. Our on-site orbital magnetization results appear to qualitatively and quantitatively differ from Bianco and Resta theory. For topological insulator, we also explain how the local orbital magnetization in finite-size systems provides an interesting dual perspective of the bulk-edge correspondence.

Electron correlation through quasiparticle embedding: from altermagnetism to topology

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Within the modelling of strongly correlated materials, the ghost Gutzwiller (gGut) framework has emerged as a versatile alternative to well established, computationally intensive approaches. gGut is a variational Ansatz which can be formulated as a local embedding. By introducing auxiliary orbitals, it can describe correlated electrons in lattices and molecules in terms of effectively non-interacting quasiparticles, resulting in an efficient and interpretable formalism. Here, we will discuss two recent gGut applications: the proposal of an interaction-driven mechanism for altermagnetism [1] and the description of topological properties in correlated materials [2]. In the former, the interplay between van Hove itinerant magnetism and local exchange interactions leads to a homogeneous altermagnetic spin ordering. In the latter, the quasiparticle picture underlying gGut allows the immediate use of markers developed for non-interacting systems to describe correlated topology. These examples show how gGut can provide transparent descriptions of correlated phenomena in terms of non-interacting quasiparticles.

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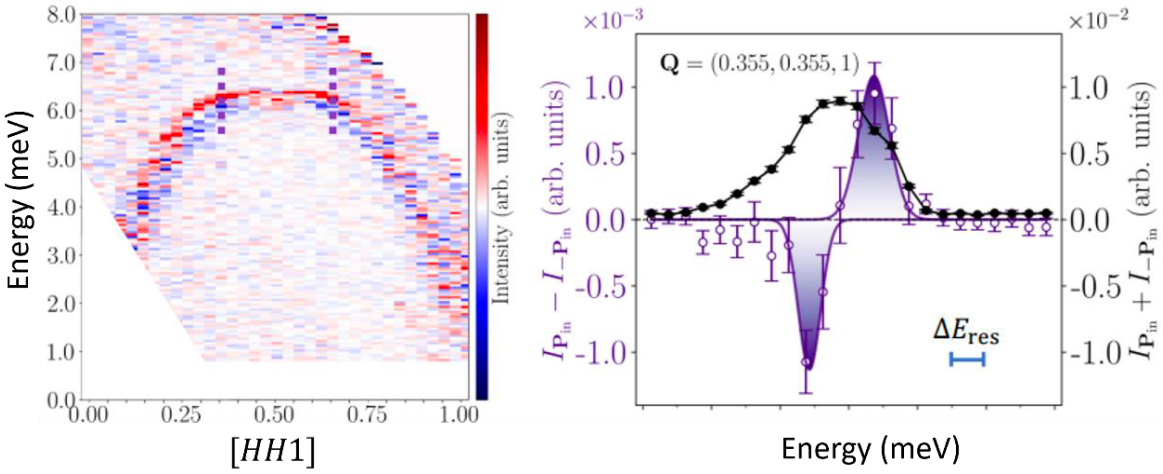
Altermagnetism revealed by polarized neutrons in MnF_2

Quentin Faure

Laboratoire Léon Brillouin, CEA-Saclay

Altermagnets (AMs) are collinear antiferromagnets in which momentum-dependent spin splitting can occur even without spin – orbit coupling [1]. Their sublattices are related not by a primitive translation but by a non-primitive translation combined with rotation, breaking time-reversal symmetry without producing net magnetization. In the magnon spectrum this leads to two branches of opposite chirality, a defining signature of altermagnetism [2].

Here, we present polarized inelastic neutron scattering (INS) results on MnF2 [3] a material long regarded as a prototypical antiferromagnet. Our data reveal a clear magnon band splitting, which we show arises predominantly from long-range dipolar interactions. Crucially, while the origin of the splitting is dipolar, the polarized INS response demonstrates a finite chirality in the cross section that reverses sign between the two branches. This persistence of chirality establishes MnF2 as an altermagnet. Our work demonstrates the unique sensitivity of polarized INS to fine magnon structure and highlights its power for identifying altermagnetic order in quantum materials.



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Recent results on Majorana chains

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The search for and interest in Majorana fermions remains an important topic. One of the simplest situations in which they can be understood, at least theoretically, is in one-dimensional (1D) Ising-Kitaev-type systems. In these models, Majorana fermions can appear as "unpaired" objects at the edges of open wires. This idea was first described by Alexei Kitaev in 2001 [1] for the transverse-field Ising chain with open boundary conditions (OBC). Then, Fendley introduced the more general and powerful notion of strong Majorana zero modes (SMZMs), which can affect the entire many-body spectrum, yielding an exact pairing between the two parity sectors at all energies [2]. In this short talk, I will start by introducing SMZMs for clean Ising-Kitaev chains and discuss recent results. First, I will present an exact calculation [3] of the SMZM fidelity FMZM, a simple topological marker that quantifies the exactness of the mapping between the two parity sectors. While FMZM takes the value 1 in the topological regime and 0 in the trivial phase, we surprisingly get the transcendental number $\mathcal{F}_{\rm MZM} = 2\sqrt{2/\pi}$ at the Ising critical point. This value turns out to be universal along the (1+1) Ising critical line, independent of the energy [3]. If time permits, I will also briefly mention various extensions and open questions, first concerning the separate effects of disorder [4] and interactions [5], as well as the interplay of both [6, 7].

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[a] Collaborations with Natalia Chepiga (Delft), Saurav Kantha (LPT), Nicolas Macé (LPT), Gabriel Lemarié (LPT).

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Doping tunable charge density waves in misfit layer compounds

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Transition metal dichalcogenides (TMDs) are a class of two-dimensional materials with unique electronic, optical, and mechanical properties, making them promising for applications in electronics, optoelectronics, and related fields [1]. In particular, $NbSe_2$ exhibits both superconductivity and charge density waves, leading to an intriguing interplay between these two electronic phenomena. Misfit layer compounds are van der Waals layered heterostructures formed by stacking layers of transition metal dichalcogenides with layers of monochalcogenides. Theoretically, it has been shown that a charge transfer occurs from the monochalcogenide layers to the TMD layers, resulting in significant doping of these layers. Furthermore, adjustment of the chemical composition of the monochalcogenide layers enables precise control over the doping level in the TMD layers. [2]. In this work, we show via scanning tunneling microscopy (STM) that in the compound $(LaxPb1-xSe)1.14(NbSe_2)_2$, the Fermi level of $NbSe_2$ can be continuously shifted from 0.0 eV up to 0.3 eV by varying the La content. Furthermore, combining STM experiments with density functional theory (DFT) calculations, we demonstrate that $NbSe_2$ undergoes a doping-induced transition from the conventional 3×3 CDW state at low doping to alternatives CDW configurations at higher doping levels. The superconducting critical temperature also varies with the shift of the Fermi level, offering a novel platform to explore the interplay between superconductivity and charge density waves in these materials.

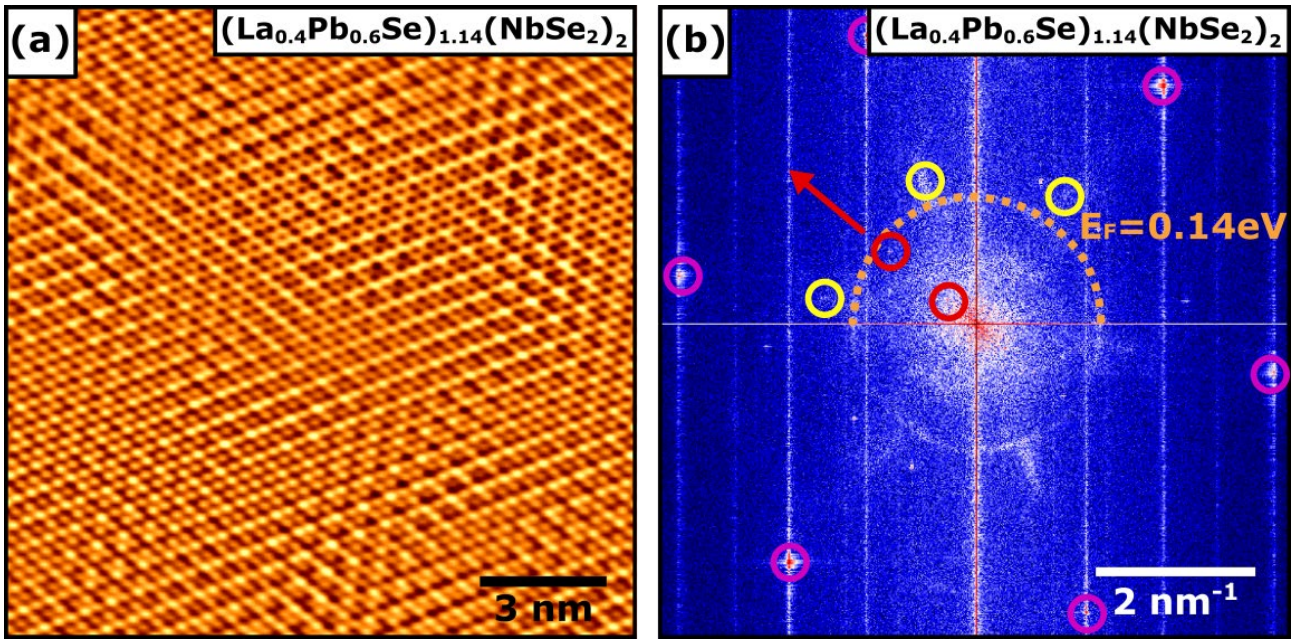

Fig. 1. a) STM image of $(La_{0.4}Pb_{0.6}Se)_{1,14}(NbSe_2)_2$ b) Associated Fourier transform exhibiting 2x2 CDW and quasiparticle interferences pattern

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Multiple magnetic transitions and coordination environments in the $MCuFe_2O_5$ (M = Mn and Co) high pressure oxides

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Charge disproportionation has been revealed among the Fe ions in $CaFe_3O_5$, leading to the formula $CaFe^{2+}Fe_2^{3+}O_5$ with a long-range collinear magnetic order below ~280 K. Nevertheless, via high-pressure and high-temperature (HPHT) synthesis, substantial differences have recently been observed when replacing Fe2+ by Cu2+ which has a strong JT response with a variety of magnetic order states below T_N = 350 K (Mn) and 300 K (Co). Combining these ideas: i) substituting Fe^{2+} by Cu^{2+} and ii) Ca by Mn or Co via HPHT synthesis in $CaFe_3O_5$, we have obtained the novel $MCuFe_2O_5$ (M = Mn and Co) oxides at 10 and 20 GPa and 1273 K with a Walker-type multianvil press. Intriguingly, $MnCuFe_2O_5$ shows a different structure than $CaCuFe_2O_5$ and $MnFe_3O_5$ (Cmcm) and crystallizes in the Pnma space group (Figure 1(a&b)). Contrarily, $CoCuFe_2O_5$ preserves the Cmcm structure. The thermal evolution of the magnetic susceptibility for $CoCuFe_2O_5$ ($MnCuFe_2O_5$) shows a sharp maximum at T_{N1} = 195 (105) K and a second transition at T_{N2} = 77 (39) K as shown in Figure 1(c). It follows a Curie-Weiss behaviour above 300 (150) K and presents a $|\theta|$ = 700 (218) K with a μ_{eff} = 5.7 (6.6) μ_B/f.u, larger than the expected value of μ_{theo} = 4.7 (5.2) μ_B/f.u. The field-dependent magnetization at 2 K of both systems indicates a ferrimagnetic arrangement. The detailed neutron measurements will be presented. Complete neutron diffraction measurements will be included to elucidate the cation ordering, along with specific heat measurements to provide further insights into the nature of the magnetic transitions.

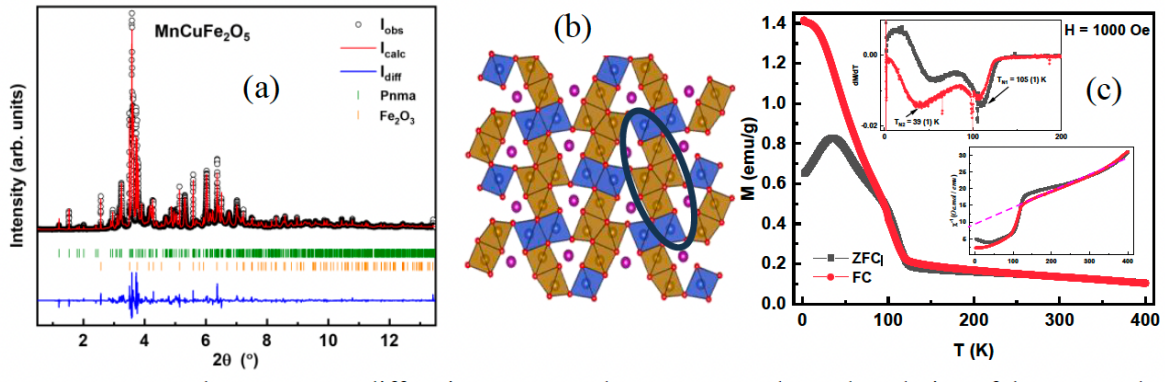

Figure 1. a) Synchrotron X-ray diffraction; **b)** Crystal structure; **c)** Thermal evolution of the ZFC and FC magnetization of high-pressure *Mn*$CuFe_2O_5$.

Nanocharacterisation of $NbSe_2$/GaP epilayers.

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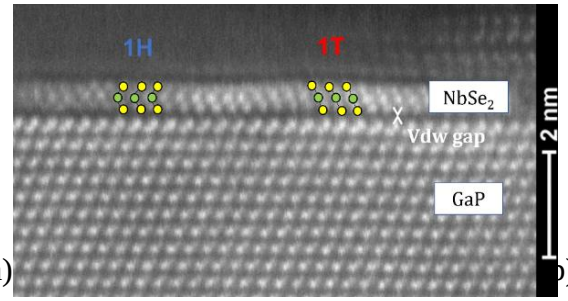
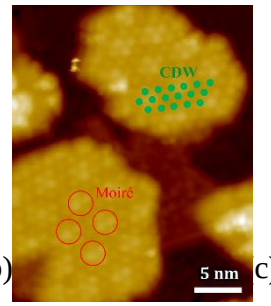
Transition metal dichalcogenide $NbSe_2$ has been extensively studied in bulk 2H phase for its superconductivity properties coexisting with a charge density wave (CDW) state. More recently, 1T-$NbSe_2$ has been synthesised by molecular beam epitaxy (MBE) and bi-dimensional Mott insulating state coexisting with a CDW as been identified [1].

This work aims at growing by MBE monolayer 1T and 1H $NbSe_2$ on a semiconducting GaP substrate as well as characterise the resulting epilayer through photoemission spectroscopy (XPS, UPS), electron diffraction (RHEED, LEED) and microscopy (STM, STEM).

The successful epitaxial growth of $NbSe_2$ is confirmed by RHEED which indicates a good surface quality although phase mixture occurs as depicted in STEM imaging where 1T and 1H domains are clearly defined (Fig. 1a). STM image (Fig. 1b) confirms the presence of both 1T and 1H domains with CDW and Moiré superstructures, also observed in LEED (Fig. 1c), attesting the substrate interaction arising in $NbSe_2$/GaP. In predominantly 1T samples, the valence band measured by UPS unveils a semiconducting behaviour with a maximum at 0.4 eV as reported by previous work on graphene substrate [1]. The quality of the obtained monolayer paves the way towards microscale and macroscale electrical measurements for future device integration.

(a) 

(b) 

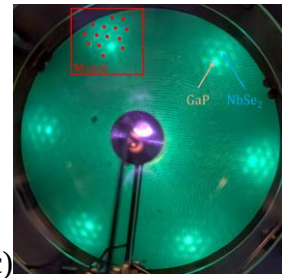
(c) 

Figure 1. (a) STEM image of the epilayer, (b) STM image with 1T and 1H domains and (c) LEED pattern showing the Moiré superperiodicity.

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Full d manifold DMFT calculation with spin-orbit coupling for Ba_2IrO_4 and Ba_2RhO_4: revisiting the TP equivalence approximation with correlations

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Accurate treatment of the d manifold in dynamical mean-field theory (DMFT) [1] is costly, particularly in systems where the e_g states can hybridize with the t_{2g} ones. Motivated by the TP equivalence approximation [2] which allows a controlled separation between the t_{2g} and e_g states, we present a layered extension of Dynamical Mean Field Theory (L-DMFT) that treats the e_g states and their coupling to the t_{2g} ones at the mean-field level. This method enables routine full d manifold calculations including spin-orbit coupling at a reduced cost while maintaining an accuracy close to a full DMFT calculations.

We apply this method to Ba_2IrO_4 and Ba_2RhO_4, two d^5 materials for which the e_g states, while being expected to be empty, lie below the Fermi level in a (PBE) density functional theory description. L-DMFT reproduces the diagonal and off-diagonal DMFT self-energies with near quantitative accuracy. Momentum resolved and integrated spectral functions reveal that the eg weight is shifted above the Fermi level, yielding a clear separation from the t_{2g} manifold.

Our results establish L-DMFT as a controlled alternative to full DMFT calculations to include the eg states in layered iridates and rhodates without sacrificing accuracy in the low-energy t_{2g} physics. Benchmarking this method on Ba_2IrO_4 and Ba_2RhO_4, we find a ~40x speedup with L-DMFT compared to a full five-band DMFT calculations. These results enable systematic d manifold studies of spin-orbit materials where the TP equivalence approximation is justified.

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Orbital-Selective Diffuse Magnetic Fluctuations in Sr_2RuO_4

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The quasi-two-dimensional Sr_2RuO_4 is a paradigmatic correlated material that becomes an unconventional superconductor at low temperatures. Although the mechanism for its superconductivity is still not fully understood, it is believed to arise from strong magnetic fluctuations. However, previous theoretical descriptions of these fluctuations have been inadequate, and significant discrepancies with experimental observations have been reported. Inelastic neutron scattering (INS) measurements reveal exceptionally strong spin excitations in this material that correspond to an incommensurate wave vector, yet no magnetic ordering has been observed in numerous experimental studies. Previous theoretical attempts, have failed to accurately describe the spin fluctuations, typically overestimating their strength and predicting the formation of an ordered state at finite temperatures. In our present work, we have elaborated a theoretical description of this multi-orbital system by self-consistently accounting for both local and non-local electronic correlations. This reduces the degree of correlations in the system, destabilizing magnetic ordering and yielding a spin susceptibility that quantitatively matches the one obtained from INS measurements. Furthermore, we show that the spin excitations in Sr_2RuO_4 exhibit an orbitally-selective character, a feature that might be linked to a multi-component superconducting state, as suggested in the literature [1].

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Neural Quantum States: Towards High accuracy, high throughput simulation of quantum matter

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Neural Quantum States (NQS) are a family of computational methods built on top of Variational Monte Carlo to tackle strongly-correlated systems. Compared to other Ab-Initio methods, NQS perform rely on no approximation, and they have shown to converge to numerically exact results for ground-states of Heisenberg antiferromagnets. More recently, several techniques to probe the entire phase diagram of such systems at a cost comparable to a single simulation have been proposed.

Three issues have been challenging researchers recently: (i) their application to molecular hamiltonians, where accurate results require unreasonable computational budgets; (ii) accessing dynamical properties, which remain challenging and (iii) when calculations fail, it is challenging to understand and diagnose why in order to improve.

In this talk I will discuss recent insights into those three problems through the lenses of Monte Carlo sampling, showing how to radically rethink VMC to lower its computational complexity by two orders of magnitude when applied to molecular hamiltonians.

I will then discuss recent progress towards accessing dynamical response functions of such systems.

Finally, I will conclude the discussion by giving general remarks about what are the successful ingredients that make this family of Scientific Machine Learning tools so successful, hopefully inspiring applications beyond what we have already done.

19 Nov 2025

Topological order at finite temperature in two dimensions

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Certain two-dimensional (2D) frustrated quantum magnets have gapped ground states and a wave-function with long-range entanglement. These are said to feature "topological order" and have fractionalized excitations with anyonic statistics. For example, the quantum dimer model on the triangular lattice is known to host a Z_2 quantum spin liquid, the fractional excitations of which are spinons and visons. A cartoon model with the same topological order is the toric code proposed in 1997 by Kitaev. A whole class of toy-models with Hamiltonians that are sums of local commuting projectors – such as the Kitaev quantum double model or the Levin-Wen string-net model – is able to generate many other types of 2D topological orders.

In this talk, we will present our recent results – obtained during the PhD thesis of Anna Ritz-Zwilling – on the finite-temperature behavior of these 2D topological orders. We have been able to analytically compute the partition function for all these models. The partition function turns out to be very similar to that of two copies of the 1D classical Potts models. As a consequence, in the thermodynamic limit, topological order is destroyed at any finite temperature. However, in a finite system, there is a finite temperature below which topological order is preserved.

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Exploring interaction-driven topological phases using a combined cluster-diagrammatic approach

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In this work, we investigate dynamical symmetry breaking in correlated electron systems, focusing on the emergence of ordered states characterized by both local and non-local order parameters. We refine the D-TRILEX formalism, which builds a diagrammatic expansion on top of an interacting reference system. By employing a cluster dynamical mean-field theory (DMFT) reference, our approach captures short-range correlations nonperturbatively, while long-range correlations are treated diagrammatically. Unlike traditional cluster DMFT extensions, which miss long-range effects, our cluster D-TRILEX scheme provides a unified framework for studying both local and non-local instabilities. We demonstrate its effectiveness on the one-dimensional Hubbard model, where non-local correlations play a dominant role and render single-site DMFT unreliable. Our results reproduce the transitions to bond-order-wave (BOW) and charge-density-wave (CDW) phases across a broad interaction range. Furthermore, the method allows us to construct an effective Hamiltonian from the self-energy, enabling a topological characterization of correlated phases. In particular, we show that the interaction-driven BOW phase exhibits topological features analogous to those of the Su–Schrieffer–Heeger (SSH) model.

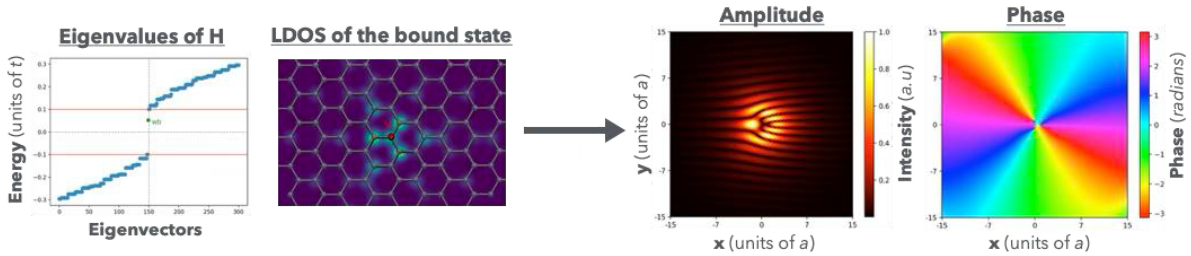
Topological study of quantum bound states in Dirac materials

Simone Reda NABIL, Pascal SIMON, Andrej MESAROS

Laboratoire de Physique des Solides (LPS) – Université Paris-Saclay

We study the local density of states (LDOS) around local impurities in two-dimensional Dirac-like electronic systems, looking for signatures of wavefunction topology. We first review the known example of a hydrogen adatom in graphene that induces resonant states whose LDOS shows oscillations with a vortex-defect in their phase, originating from the topological winding of the phase of the Bloch wavefunctions around the Dirac points [1,2].

We then extend this framework to gapped systems such as hexagonal boron nitride (hBN), and spinful models with Kane-Mele and Valley-Zeeman spin-orbit couplings, where the impurity gives rise to exponentially localized bound states within the gap. These states provide a direct spatial signal accessible via STM measurements, allowing us to extract topological features in the amplitude and phase of the wavefunction (see the Figures below).



These extensions are relevant for impurities in transition metal dichalcogenides (TMDs) materials. The resulting LDOS retains angular modulations whose features depend on spin, valley, and impurity strength. Our results highlight that the LDOS around a defect does reflect some topological features, but that the correlation to the Berry phase is not always direct—particularly in models with a semi-Dirac dispersion.

Altogether, these findings demonstrate that impurity-induced LDOS patterns offer a versatile probe of wavefunction topology. Our goal is to apply this theoretical framework to STM measurements on real TMD materials, enabling a real comparison between observed LDOS features and theoretical predictions.

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Quantum kinetic equation approach to thermal Hall conductivity with disorder

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I will present a systematic derivation of the semi-classical kinetic equation for neutral bosons from their quantum kinetic equation. It incorporates the semi-classical topological dynamics of wave packets in the form of geometric properties of the energy eigenstates, such as the Berry connections and curvatures, generalized to phase space. This makes it possible to treat inhomogeneous systems, including boundaries, textures, etc., in a compact and natural manner, and to compute the associated observable quantities, such as energy and current densities, away from equilibrium. In particular, this provides a self-contained rigorous derivation of the intrinsic thermal Hall effect, avoiding subtleties associated with magnetization currents. I will then show how this formalism allows to efficiently include extrinsic effects, such as the coordinate shift contributions in the presence of disorder.

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Presentation type : [oral OR poster] Oral *Choisissez un élément.*
I authorize the GDR to record a video of my presentation : [Yes OR No] Yes

Photoinduced Phase Dynamics in Morphologically Tailored Transition Metal Oxides

The ability to control light–matter interaction in quantum materials offers a pathway to access and stabilise non-equilibrium states with emergent functionalities not attainable under thermal equilibrium[1, 2]. Ultrafast laser excitation can indeed drive phase transitions in materials exhibiting strong coupling between electronic and structural degrees of freedom - particularly those involving large volume changes associated or not to a symmetry breaking [3, 4]. Recently, the effect of nanoscopic morphology has been observed on both the mechanism of macroscopic transformation and the thermal relaxation process [5]. However, a complete understanding of the impact of morphology on the dynamics and efficiency of such transformations is still lacking and hence stands as an important emerging area of research.

In this work, we investigate the ultrafast structural dynamics in morphologically tailored transition metal oxides, focusing on vanadium sesquioxide (V_2 O_3) and trititanium pentoxide (Ti_3O_5) systems, including polycrystalline thin films and single crystals prepared via Focused Ion Beam (FIB) technique. Using time-resolved X-ray diffraction, we track the evolution of transient phases following laser excitation and compare the dynamics across different geometries and crystallographic orientations.

These findings underscore the critical role of nanoscale morphology in dictating photoinduced phase dynamics in the ps-ns range and offer design principles for engineering ultrafast devices based on transition metal oxides with controllable non-equilibrium functionalities.

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Symmetry manipulation of Floquet-Bloch states

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Centre Lasers Intenses et Applications (CELIA)

Driving quantum materials out of equilibrium enables the creation of states of matter that are inaccessible through conventional equilibrium tuning methods. When electrons are coherently driven by time-periodic electromagnetic fields, hybrid light–matter states (known as Floquet–Bloch states) emerge, offering new routes for the generation and control of exotic light-driven quantum phases. It has been predicted that by tailoring the polarization state of the driving field, one can imprint specific symmetry properties onto these photon-dressed electronic states. In this talk, I will discuss the experimental exploration of symmetry-guided selection rules in Floquet–Bloch engineering of two-dimensional materials using time- and angle-resolved photoemission spectroscopy. First, we will look at transition metal dichalcogenides, where broken inversion symmetry within each monolayer produces a non-zero Berry curvature at the K and K' valleys, giving rise to chiroptical selection rules central to valleytronics. We demonstrate the formation of valley-polarized Floquet–Bloch states in 2H-WSe_2 under sub-bandgap coherent driving with circularly-polarized light pulses [1]. Moreover, extreme ultraviolet photoemission circular dichroism in this nonequilibrium regime reveals the ability to manipulate the orbital character of Floquet engineered states. Second, in nonsymmorphic SnS, we show that the photon-dressed sidebands exhibit polarization-resolved photoemission intensities opposite to those of the valence band at the Brillouin zone edges. This behavior indicates a light-induced parity inversion of the electronic wavefunction of Floquet engineered states. Together, these results highlight the potential of light fields to induce symmetry-controlled nonequilibrium electronic structures of 2D materials, opening pathways toward the design of novel light-induced quantum phases of matter.

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CDW phase under an electric field observed by an XFEL source

David Le Bolloc'h

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Under an external applied field, an incommensurate Charge Density Wave (CDW) may slide leading to the appearance of an excess of current. The atomic lattice is directly involved in the transport process [1]. Indeed, the collective current is linked to structural changes in the periodic lattice distortion associated with the CDW. Above the threshold field, longitudinal deformation is observed with compression of the CDW modulation near one electrode and expansion near the other [2]. Other studies have shown that a large transverse deformation is also present below the threshold, which can be explained by strong pinning by the sample surfaces [3]. To better understand this sliding phenomenon, the CDW deformation has been observed in $NbSe_3$, under an electric field, using a coherent XFEL source in order to retrieve the CDW phase.

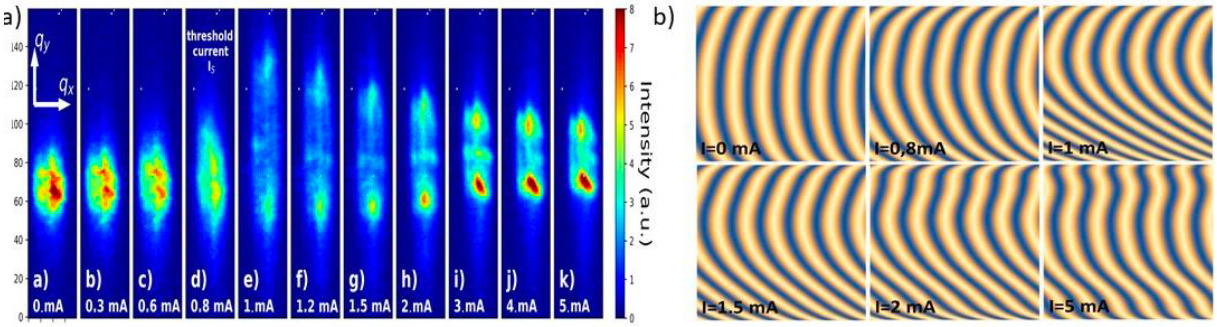

Figure 1: a) Diffraction experiment performed at LCLS: Q(0 1.241 0) satellite reflection associated to the CDW in $NbSe_3$ with increasing currents (T=80K). b) Corresponding CDW obtained from the diffraction patterns.

We used a genetic algorithm to retrieve the CDW phase from diffracted intensities. A balance between the two types of deformation is observed. For currents below threshold, increasing shear deformation is observed in the central part of the sample while longitudinal deformation appears above threshold when shear relaxes. Shear thus precedes longitudinal deformation, with relaxation of one leading to the appearance of the other. Moreover, strain accumulates on surface steps in the sliding regime, demonstrating the strong pinning character of these surface discontinuities. Sliding processes are thus based on CDW which, despite its nanometric wavelength, involves the entire (macroscopic) sample. This study also shows that the excess current is due to nonlinearities induced by CDW deformations [4].

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Contrôle de l'ordre onde de densité de charge de $ErTe_3$ par la contrainte uniaxe

Théotime Freitas[1], Mattia Udina[1], Alexis Lespinas[1], Alexandr Alekhin[1], Niloufar Nilforoushan[1], Sarah Houver[1], Alain Sacuto[1], Benito Gonzalez[2], Ian Fisher[2], Indranil Paul[1] et Yann Gallais[1]

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Les matériaux quantiques ou les systèmes à forte corrélations électronique présentent de nombreux ordres électroniques complexes, généralement en compétition, tels que la supraconductivité, le magnétisme et les ordres de charges. Les tritellures de terre rare RTe_3 (avec R=Y, La-Nd, Sm, Gd-Tm) de structure orthorhombique sont des composés onde de densité de charge (CDW) paradigmatiques possédant 1 ou 2 ordres CDW 1Q quasi-dégénérés et possédant des orientations orthogonales [1]. La direction de la modulation 1Q-CDW est dictée par une faible anisotropie structurale associée à un plan de glissement [2].

Dans mon exposé je présenterai des mesures de spectroscopie Raman couplée à un dispositif de contrainte uniaxe réalisées sur le composé ErTe3. Je montrerai que l'anisotropie du mode d'amplitude CDW observée en Raman peut être utilisée pour déterminer l'orientation de l'ordre CDW. Je mettrai ensuite en évidence le renversement contrôlé de l'orientation de la CDW par la contrainte uniaxe. Finalement je discuterai de la présence inattendue d'une distorsion monoclinique unique à l'état 1Q-CDW et suggérant un ordre plus complexe qu'initialement anticipé.

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20 Nov 2025

Towards a minimalist description of strange metals

Simone Fratini

Institut Néel, CNRS, Grenoble

After reviewing recent exact numerical results on the transport and optical response of the t-J and Hubbard models, I will introduce an analytical theory of transport in quantum materials that is based on the assumption that the motion of the charge carriers obeys the correspondence principle, in the sense that the quantum mechanically averaged carrier diffusion in time is analogous to the classical case. I will show that in bad metals, where wave-like coherence is lost at each hop between neighboring atoms or molecules, this assumption naturally leads to strange T -linear resistivities with apparently Planckian scattering rates as well as both the stretched Drude and displaced Drude peaks that are commonly observed in optical absorption experiments. The present framework might also help understanding the broad, dispersionless collective modes observed through RIXS and M-EELS in the cuprates, and indicate a solution to the problem of universal dielectric relaxation in insulators.

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Non-Local Correlation Effects in DC and Optical Conductivity of the Hubbard Model

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The Many-body effects in correlated materials can be explored through various response functions, with transport measurements being among the simplest and most direct probes. However, despite the apparent simplicity of these experiments, a reliable theoretical framework for accurately interpreting their results remains elusive. Remarkably, even the single-band Hubbard model, which is the minimal model that captures the interplay between electron kinetics on a lattice and on-site Coulomb repulsion, presents significant challenges for the theoretical calculation of transport properties.

Accurately addressing the unconventional transport properties of materials requires accounting for spatial electronic correlations. These correlations can significantly influence transport properties by modifying the electronic spectral function and giving rise to complex multi-electron scattering processes, known as vertex corrections, which can strongly impact the conductivity. Incorporating non-local vertex corrections in state-of-the art methods remains a major computational challenge. For this reason, the effect of spatial correlations on transport properties is largely unexplored, due to the lack of appropriate theoretical tools

In this talk, based on our recent work [arXiv:2507.16673], I will discuss the impact of non-local correlations on the conductivity of the single-band Hubbard model within the recently developed Dual GW (D-GW) [PRB **111**, 235129 (2025)] approach. This method enables a consistent real-time description of local electronic correlations and long-range collective charge and spin fluctuations across weak- and strong-coupling regimes, offering direct access to single- and two-particle observables in real frequencies. By focusing on the region near the Mott transition, I will demonstrate that the impact of non-local correlations on the conductivity differs between the correlated metallic and Mott insulating phases. I will show that incorporating nonlocal correlations in both the electronic spectral function and vertex corrections is crucial for accurately describing the DC and optical conductivity in the metallic phase. The crossover between the metallic and Mott insulating phases is marked by a vanishing contribution of vertex corrections to the DC conductivity, although the DC conductivity itself remains finite at high temperatures. At the same time, non-local vertex corrections remain essential for describing the optical conductivity in the Mott insulating regime, despite the fact that this regime is dominated by local electronic correlations.

Slave Spin Study of the Mott Transition and Antiferromagnetism in the 2D Hubbard Model

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We study the two-dimensional Hubbard model using the slave spin mean field approach [1-3], focusing on how lattice geometry influences the physics of correlated electrons. This method provides a computationally efficient framework for exploring both para-magnetic [1-3], and antiferromagnetic phases [4]. We also introduce frustration by including next-nearest-neighbor hopping (t') to examine its effects on both the para-magnetic and antiferromagnetic phases. Our analysis shows that, in the paramagnetic regime, the method reveals the dependence of the critical interaction strength of the Mott metal-insulator transition on lattice geometry. In the antiferromagnetic regime, it further clarifies the interplay between electronic correlations and magnetic order. Building on these results, we are extending the study to multiorbital systems, with calculations currently in progress. These findings highlight the versatility of the slave spin approach in addressing the complex behavior of strongly correlated electron systems.

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Far-field and near-field optical spectroscopy to probe correlated materials

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GREMAN UMR7347 - Université de Tours, CNRS, INSA CVL

Optical spectroscopy is a powerful and versatile tool for investigating both the electronic and vibrational properties of strongly correlated systems, where the collective behavior of electrons gives rise to exotic phenomena [1]. One of its key advantages lies in its compatibility with diverse experimental environments, allowing for the precise tuning and control of a material's electronic, structural or magnetic phases using external stimuli like temperature, pressure, light, electric field, ... This capability is very useful for mapping complex phase diagrams and uncovering the physics behind phenomena such as metal-insulator transitions (MITs). Here, we employ optical spectroscopy to explore to study the evolution of electronic properties in a variety of materials, including oxides, chalcogenides, organic compounds.

However, a major drawback of conventional optical spectroscopy is its spatial resolution, which is limited to tens of microns in the infrared spectral range. Scattering-type Scanning Near-field Optical Microscopy (s-SNOM) is able to overcome this fundamental barrier and unlock a new dimension of nanoscale characterization [2,3]. This relatively recent technique uses a sharp atomic force microscope (AFM) tip to locally probe the evanescent field at the illuminated sample surface, which allows to break the diffraction limit and achieve a nanoscale resolution of a few tens of nanometers. This capability allows for both imaging and spectroscopy of inhomogeneities in electronic or vibrational properties. For instance, it can be used to visualize phase separation or electric-field-induced conductive nano-filaments in Mott insulators, composite materials, ... Furthermore, s-SNOM is invaluable for studying very thin or quasi-2D materials, like ferroelectric freestanding membranes or artificial moiré superlattices.

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Propagation of nanoscale metal-insulator domain walls in Cr – V_2O_3 systems tracked through *in situ* electron spectromicroscopy techniques

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Taming abrupt resistive transitions in correlated materials such as $(V_{1-x}Cr_x)_2O_3$ requires a detailed understanding of the local mechanisms governing the dynamics of electronic phase separation at the metal-insulator transition (MIT) [1]. While the T-driven MIT in Cr-doped V2O3 has been extensively studied at the macroscopic scale mapping the dynamics of nanoscale switching remains challenging, especially when relying on separate structural and spectroscopic probes [2,3,4]. This underscores the need for combined in situ investigations within a single instrument.

In this work, we exploit advanced monochromated electron spectromicroscopy to correlate, at the nanometer scale, local electronic excitations — captured with ultra-high energy resolution electron energy-loss spectroscopy (EELS) — with structural features revealed by 4D STEM microdiffraction during low-temperature thermal cycling. More recently, we employed a Timepix3 direct electron detector operated in event-based mode, enabling the recording of individual electron arrivals with precise timing and energy information. This allowed us to perform time-resolved low-loss EELS measurements at the millisecond scale, giving direct access to the dynamics of nanoscale electronic phase separation and shedding new light on the local mechanisms driving the MIT.

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Competing and cooperating orders in UTe_2

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Superconductivity in UTe_2 has many striking properties, like extremely high and anisotropic critical fields and the existence of multiple superconducting phases induced by either pressure or magnetic field. However perhaps the most unusual feature is the reinforcement of superconductivity in applied magnetic fields. The usual effect of magnetic field on superconductivity is through the effect of the field on the motion or the spin of the carriers. The effect of magnetic field on the pairing mechanism is absent or negligeable. This is not surprising in conventional superconductors where the pairing mechanism stems from the electron-phonon interaction, but it is also the case in most unconventional superconductors, even when the pairing mechanism has a magnetic origin. UTe_2 is one of the few exceptions where an applied magnetic field can enhance the strength of the pairing mechanism and actually reinforce superconductivity. In ambient pressure conditions, this effect is most spectacular when the field is applied along the b-axis of this orthorhombic system, where, above 15T, the superconducting critical temperature increases with increasing field. However under pressure a reinforcement of superconductivity with magnetic field is found for field applied along the c-axis. In both cases the probable origin is the proximity of a magnetic phase transition line that can be crossed by tuning the field. For H//b this is the metamagnetic transition to a polarized state at about 35T. Under pressure, two further transitions have been detected: a transition to a long-range antiferromagnetic state, and a second transition to a so far unidentified state. We present new results under pressure which help to clarify the role of these different transitions in helping or hindering superconductivity in UTe_2.

Paramagnetic limit of spin-triplet superconductors

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The overcome of the conventional s-wave paramagnetic limit [1,2] is usually interpreted as an indication of unconventional superconducting pairing, for example characterized by spin-triplet pairing. However, a rigorous treatment of the spin-triplet paramagnetic limit itself is lacking. Here, we study the phase diagram of spin-triplet superconductors, considering the effect of the external magnetic field on the electrons' spins [3]. For a given symmetry of the order parameter and a generic orientation of the field, the paramagnetic limit for superconductivity diverges at low temperatures. For specific directions of the field, we identify a range of temperatures where the transition between normal and superconducting phases becomes of the first order. When two tricritical points exist along the transition line, a first-order phase transition between two superconducting phases may develop in vicinity of the tricritical point with lower temperature. We discuss the implications of our findings for the anisotropy of the upper critical field in UPt_3, a candidate material for triplet superconductivity, when both the paramagnetic and orbital effects are taken into account.

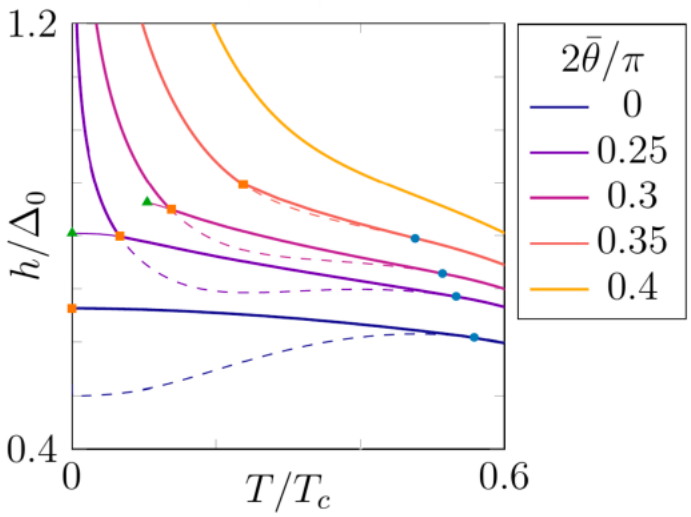

Fig. 1 : Paramagnetic upper critical field vs. temperature at different angles of the Zeeman magnetic field, for an order parameter of the type $d(k) \sim (0\ 0\ k_z)$. Tricritical points are represented by blue circles and orange squares, critical points are represented by green triangles. It also shows the upper critical line at the second-order transition (dashed line) and the critical line at the first-order transition inside the superconducting phase (thin line).

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Electrostatic Control of Superconductivity in $KTaO_3$-2DEG in top-gate devices.

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The search for Majorana fermions has become one of the most exciting topics in quantum materials, since they could enable fault-tolerant topological quantum computing. Many platforms have been suggested, but experiments remain difficult because the materials must combine strong superconductivity with strong spin–orbit coupling.

Oxide heterostructures are especially promising because they naturally bring these ingredients together. After decades of work on $LaAlO_3/SrTiO_3$ systems, a major breakthrough came with the discovery of superconductivity in (111)-oriented $KTaO_3$ heterostructures. These systems reach critical temperatures of 2.2 K — almost ten times higher than $SrTiO_3$ interfaces. On top of that, the heavy tantalum atoms give much stronger spin–orbit coupling, making $KTaO_3$ a very attractive platform to explore topological superconductivity.

In this work, we demonstrate for the first time local electrostatic control of superconductivity in a two-dimensional electron gas (2DEG) at the $KTaO_3$(111)/AlOx interface by employing top gates with an HfO_2 dielectric. Unlike global modulation via a back gate, the top gate enables spatially selective tuning of superconducting properties, a crucial capability for fabricating functional quantum circuits. Systematic transport measurements under varying gate voltages reveal a superconductor–insulator transition (SIT) up to 2.2 K.

By mapping the gate-voltage–temperature parameter space, we derive a detailed phase diagram that uncovers a quantum critical point separating superconducting and insulating regimes, with scaling behavior characteristic of two-dimensional quantum phase transitions. The device operates as a gate-tunable superconducting transistor, offering reversible control over the SIT. These findings establish a versatile platform for locally defined Josephson junctions and SQUIDs based on oxide interfaces, paving the way for engineering complex superconducting quantum circuits and exploring topological superconductivity in oxide heterostructures.

Evidence of homogeneous superconductivity in the strongly overdoped regime of $YBa_2Cu_3O_{7+x}$ up to $x \sim 0.5$

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In recent years, there has been growing evidence that high-T_c superconductivity in cuprates can persist in the overdoped region at doping levels up to $p \sim 0.5$ hole/Cu, well beyond the superconducting dome previously established, where a Fermi liquid phase is rather expected. Previous reports concern high-pressure oxygenated $YBa_2Cu_3O_{7+x}$ for x up to 0.5 [1,2], $(Cu_{0.75}Mo_{0.25})Sr_2YCu_2O_{7+x}$ [3], for $x \sim 0.54$, corresponding to $p \sim 0.46$ hole/Cu, a high-pressure compound, $Ba_2CuO_{3.2}$, for $p \sim 0.4$ hole/Cu [4] and thin $La_{2-x}Ca_xCuO_4$ films for $x = 0.4$ [5]. These results put into question the widely accepted picture that superconductivity vanishes at $p \sim 0.27$-0.30 hole/Cu. The decrease of superfluid density in the overdoped region ('boomerang effect' [6]), while the electronic specific heat, γ, increases [3] suggests a scenario of electronic phase separation between normal and superconducting holes [7].

In order to elucidate the above question, here we report on the reproducible synthesis of single-phase $YBa_2Cu_3O_{7+x}$ samples where strong overdoping up to $x \sim 0.4$ has been achieved by means of high-pressure oxygenation. Our Rietveld refinements of X-ray and neutron diffraction data show that sample purity is 95% or better and that the *a*-axis parameter progressively increases with *x*, while the *c*-axis progressively decreases, consistent with an increase of the occupancy of the oxygen site in the CuO plane. In agreement with previous reports, the T_c onset is only slightly reduced as compared to optimally doped samples, while the superconducting transition broadens significantly. Contrary to other overdoped compounds, γ vanishes, which rules out electronic phase separation and rather suggests a picture of homogeneous superconducting phase where all extra holes contribute to the superconducting density. The challenge is therefore to explain the weak sensitivity of T_c on hole density in the strongly overdoped region.

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Disorder as a new tool to design original geometrically frustrated magnetic materials

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High entropy oxides are a new family of materials born from the revolutionary approach proposed by Rost *et al*. in 2015 [1] and have since aroused considerable interest. These oxides are characterized by a large number of cations introduced on one or several sub-lattices, giving rise to a high configurational entropy. Among these materials, there is a special case called entropy-stabilized oxide, in which the entropy term ($T\Delta S$) becomes preponderant in the free energy above a critical temperature ($\Delta G = \Delta H - T\Delta S$), overcomes an unfavorable enthalpy of formation and drive the system to a single phase, allowing some cations to be stabilized in unusual configurations (valence state, coordination and structural environment). This opens a new route for material design and allows one to create new versatile compounds with highly tunable and unique physical properties.

Recently, by combining the high-entropy concept with structures allowing geometrically derived magnetic frustration, we have designed and synthesized several original compounds, including the first entropy-stabilized oxide with a pyrochlore structure ($A_2B_2O_7$) [2, 3]. This new approach of materials design allows more precise adjustment of the chemical pressure, gives access to an incredible number of new compositions, and provides a new tool for probing magnetic behavior [4].

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MAGNETIC PHASES AND ZONE FOLDED PHONONS IN A BULK FRUSTRATED VAN DER WAALS MAGNET

Two-dimensional (2D) magnetic materials have attracted extensive research interest due to their potential applications in fields such as nanospintronics and optospintronics [1], and because of their importance in fundamental physics. For instance, on-lattice frustration can result in a variety of magnetic phases, which can be investigated by varying the temperature, magnetic field, or hydrostatic pressure.

In such materials, magnetoelastic interactions allow to use magneto-optical spectroscopies to follow the phase diagram. In this context, magneto-Raman spectroscopy has emerged as the method of choice. It has been particularly useful in probing magnetic transitions and couplings in 2D antiferromagnets such as $MnPS_3$ [2,3] or $FePS_3$ [4].

CrOCl is a frustrated 2D antiferromagnet with a rich magnetic phase diagram and its magnetic transitions are visible in its Raman spectra: as a magnetic field is applied, low-intensity Raman modes appear and disappear as transitions occur between magnetic phases.

In this study, we used density functional theory (DFT) based methods to calculate the phonon modes and their Raman intensities. These calculations allowed us to gain insight into the Raman spectra of CrOCl and its magnetic phases. We showed that different magnetic orders induce small lattice distortions that change the size of the unit cell, effectively resulting in multiples of the primitive cell size. In this context, we showed that the low intensity lattice vibrations that appear or disappear in the Raman spectra are directly related to changes in periodicity of the magnetic phases. Finally, we have used an "unfolding" theoretical procedure to find the connection between the low intensity modes and the phonon band structure of the paramagnetic phase [5].

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From Classical Spin-Liquid Classification to the Engineering of Pinch Lines and High-Rank Half-Moon Systems

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In recent years, numerous works have advanced the classification of classical spin liquids, proposing theoretical systems that exhibit truly exotic features [1,2]. Among these are multifold pinch points observed in structure factors, signaling emergent Coulomb physics that extends beyond the familiar spin-ice paradigm [3]. Instead of divergenceless vectors, these systems exhibit tensor-based constraints, leading to the emergence of fractonic charges—exotic quasiparticles with subdimensional mobility emerging from a tensorial form of electromagnetism. Among them are pinch-line models, where pinch points extend along one-dimensional singularities [4]. However, the occurrence of pinch lines remains rare, leaving their underlying physics only partially understood.

Here, we introduce a simple recipe for designing 3D classical spin systems that host pinch lines, enabling a diverse array of realizations [5]. We reveal a new class of pinch lines whose pinch-point structure continuously evolves along the line—unprecedented in previous models. This behavior can be captured in a general framework where two-dimensional electric fields (of possibly distinct ranks) interfere along the pinch line, illustrating the potential coexistence of multiple forms of generalized electromagnetism within a single system.

Then, we use flat-band engineering methods in order to stabilize the above-mentioned gauge charges in the ground state, rendering the spin-liquid phase an excitation [6]. Adding cluster–cluster interactions, we show that the spin liquid persists up to a critical value, beyond which pinch points are replaced by half-moon patterns. Any cluster system presenting a rank-n classical spin liquid can thus be tuned into one exhibiting multifold half moons, a signature of fractonic matter in the ground state. Further increasing the interaction strength drives a Lifshitz-type transition in analogy with the topological change of Fermi surface in the electronic structure of certain materials.

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Nanoscale Non-Volatile Filament in $(V_{0.95}Cr_{0.05})_2O_3$ Mott insulator probed by Scattering Near-Field Optical Microscopy (s-SNOM)

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Quantum Materials challenge our fundamental understanding of solids since their essential properties can be described neither by semiclassical methods nor low-level quantum mechanics. Beyond their theoretical interest, these materials also hold promise for a new generation of electronic and photonic devices [1]. Nowadays, both volatile and non-volatile resistive switching induced by electric pulses [2,3] are investigated, targeting resistive random-access memories and emerging technologies, such as optoelectronics, neuromorphic computation, actuators, sensors, logic devices. In many oxides, resistive switching can be driven by the formation of conductive filament. The insulator-to-metal transition (IMT) is triggered by strong electric fields (order of magnitude in kV/cm), which promote the electro-diffusion of either cations from the electrodes or oxygen vacancies in the oxide [2]. However, in strongly correlated materials such as Mott insulators, including chalcogenides, vanadates, and rare-earth nickelates, the IMT is governed by a local Mott electronic phase transition: the electric Mott transition at lower electric field. Understanding and controlling this IMT in Mott insulators has gathered considerable attention due to its fascinating physics and its potential technological applications in Mottronics, a new field of microelectronics based on the electric Mott transition.

In $(V_{0.95}Cr_{0.05})_2O_3$ thin films, we were able to map non-volatile conductive nanoscale filaments created by electric pulse-induced insulator-to-metal (IMT) transition at room temperature. Although no morphological or chemical changes were detected by scanning electron microscope (SEM), energy dispersive X-ray (EDX), and atomic force microscopy (AFM) after non-volatile IMT, scattering-scanning near-field optical microscopy (s-SNOM) clearly revealed the presence of a conductive filament. The shape of the filament depends on several parameters such as electric field, and pulse duration. s-SNOM measurements were performed on both parallel and tip shaped electrodes geometries, confirming that filament formation is driven by the applied electric field rather than by the electrode geometry or inter-electrode distance. We demonstrate the possibility of creating a wide range of non-volatile filaments in size and metallicity by applying different electric pulses. Importantly, the changes in s-SNOM spectra may be explained by a compressive stress within the nano-filament. The s-SNOM spectra were simulated within the framework of Finite Dipole Model [4]. We found that the infrared properties within the filament are very similar to those obtained under pressure from far-field optical spectroscopy on a $(V_{0.95}Cr_{0.05})_2O_3$ single crystal.

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Interplay of unconventional superconductivity and magnetism at cuprate–manganite interfaces

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The competition and cooperation between electronic correlations and proximity effects can give rise to emergent quantum phases at oxide interfaces. Motivated by recent experiments on cuprate–manganite heterostructures, we investigate the interplay between ferromagnetism and superconductivity within a bilayer Hubbard model solved using cluster dynamical mean-field theory. We find that interfacial magnetism can be unexpectedly reinforced by superconductivity, exceeding Pauli-limit expectations. This coexistence arises from the emergence of a triplet odd-frequency pairing component, which enhances magnetic moments on the copper sites. At stronger interfacial magnetization—such as induced by increasing the manganite thickness—superconductivity is suppressed and replaced by a correlated normal state. Remarkably, this phase combines reduced magnetic moments with a pseudogap, realizing a novel *magnetic pseudogap state*.

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Cation Distributions and Delocalization Mechanisms in Layered Monophosphate Tungsten Bronzes (L-MPTBs)

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The recently discovered series of layered monophosphate tungsten bronzes (L-MPTBs), $Ba(PO_4)_2W_mO_{3m-3}$ (m = 2–5, W^{5+}/W^{6+} mixed valence), provides a versatile framework for designing original two-dimensional (2D) electronic materials. Their structure combines $[Ba(PO_4)_2]^{2-}$ spacers with perovskite-like tungsten-oxide slabs, yielding robust metallicity and avoiding charge-density-wave instabilities thanks to their inherent "trigonality." This makes L-MPTBs ideal systems for probing and tuning 2D electron confinement through targeted cationic substitution. [1]

In these materials, edge W-sites, off-centered by PO_4 groups, can host d^0 cations or delocalized mixed-valence ions, while central high-symmetry W-sites accommodate d^n ions with delocalized electrons. Although redox stability suggests that Ta and Nb are largely confined to external sites, limiting their participation in metallic delocalization, cationic substitution in m = 2 and 3 bronzes significantly impact site preferences and electronic behavior. For m = 2, we synthesized $Ba(PO_4)_2Nb_2O_3$ and $Ba(PO_4)_2Ta_2O_3$, providing a foundation for expanding this family to more complex compositions and intergrowth structures. [2] For m = 3, we investigated $Ba(PO_4)_2W_{3-x}M_xO_6$ (M = Nb, Ta), where W-doping strongly modifies the framework, influencing electron delocalization and lattice distortions.

This strategy offers routes to confine carriers further, induce ordering effects, or trigger CDW-like instabilities. Initial results indicate that targeted substitutions influence electron localization and transport, while ongoing studies aim to explore their magnetic and electronic properties.

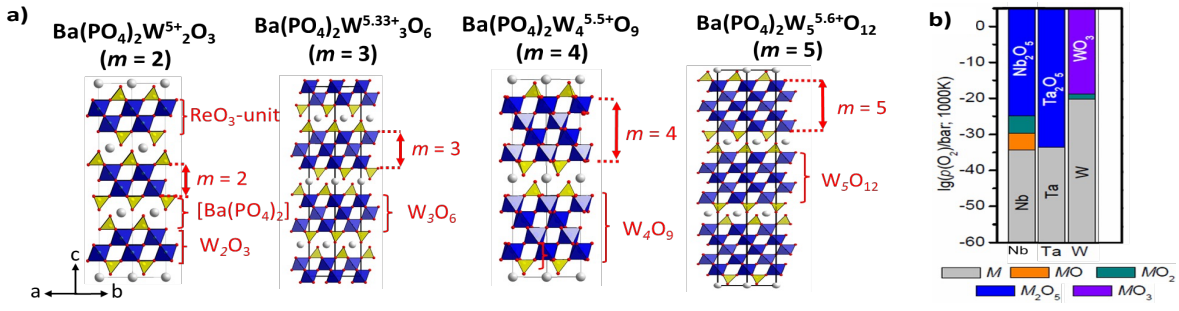

Figure 1:*Crystal structures of the L-MPTB series. b) Ellingham diagram for Ta, W and Nb at 1000K.*

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Presentation type : [oral OR poster] *Choisissez un élément. poster*
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Pressure induced ferromagnetic to antiferromagnetic transition in transition metal chalcogenide Cr_3Te_4

Transition metal chalcogenides have sparked significant attention because of their application in spintronics and magnetic storage devices. Cr_3Te_4 crystalizes in the monoclinic structure. It is a room-temperature soft ferromagnet with alternating stacks of Cr-filled and Cr-vacant layers along the c-direction. High-quality single crystals of Cr_3Te_4 were grown using the chemical vapor transport method. High-pressure XRD measurements were carried out at the PETRA P02.2 beamline with a wavelength λ=0.2910 Å. A piston-cylinder type diamond anvil cell (DAC) was used to perform the high-pressure Raman measurements with an excitation wavelength of 488 nm. The low-temperature Raman measurements were carried out using a closed-cycle helium cryostat coupled with a micro-raman spectrometer with 532 nm laser wavelength.

The ambient Raman spectra of Cr_3Te_4 consist of two major peaks arising from the in-plane and out-of-plane vibration of the Te atom. Upon increasing the pressure the peak centered around 125cm^{-1} shows red shift and the peak centered around 142cm^{-1} shows blueshift. The Raman shift of both peaks show anomaly around 7.8GPa pressure.

To investigate the possibility of any structural transition We have carried out high-pressure synchrotron XRD up to 30GPa. The ambient XRD pattern is indexed to monoclinic structure with space group C2/m. There is an isostructural transition happening around 17GPa. Since no structural transition is observed around 7.8GPa, the anomalies obtained in the Raman data around that pressure can be attributed to electronic or magnetic transition. To understand the effect of magnetic transition on the lattice vibration of the sample we have carried out low-temperature Raman measurement from 22 K to room temperature. The Raman shift of both the peaks show blue shift upon decreasing temperature up to the Neel temperature, below that softening of both the peaks observed. We have fitted three phonon decay model to eliminate the effect of anharmonicity, and it fits well up to 100 K. The deviation of experimental data below 100 K can be due to the spin-phonon coupling happening in the system. This suggests that the anomalies observed around 7.8 GPa can be due to change in magnetic ordering in the system. To confirm this DFT calculations were carried out. DFT calculations reveal the magnetic ground state changes from ferromagnetic state to antiferromagnetic state above 7.6 GPa. These findings reveal a pressure induced modification in magnetic structure and the presence of magneto-elastic coupling in Cr_3Te_4.

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Charge Density Waves in $GdTe_3$ studied by X-rays under biaxial tensile stress

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Rare-earth tritellurides (RTe_3) compounds are quasi-2D layered materials displaying incommensurate CDW (Fig.1). Concerning their crystal structure the weakly orthorhombic unit cell is along ***b*** made of two RTe_3 layers, each layer consists in a RTe slab sandwiched between two Te planes with b ≈ 25.5 Å and the (***a***,***c***) plane is nearly squared a ≈ c ≈ 4.3 Å with c/a ≈ 1.001 [1]. They are particularly sensitive to strain, and we used one of our homemade biaxial tensile stress devices based on a deformable kapton cross-shaped substrate to stretch the lattice and probe the CDW transitions by XRD in $GdTe_3$, at temperature for which only the CDW along c exists in the pristine state.

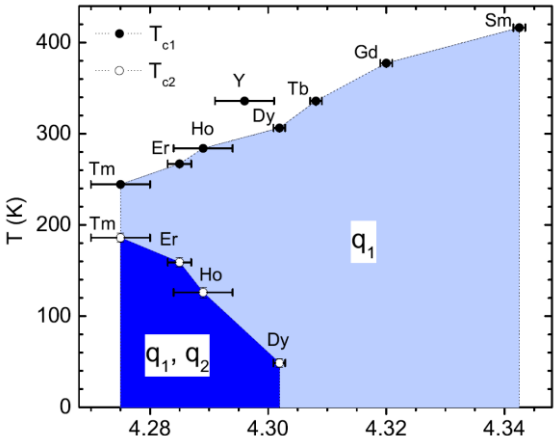

Figure 1: The CDW transition temperatures for RTe3 compounds [from ref. 1]

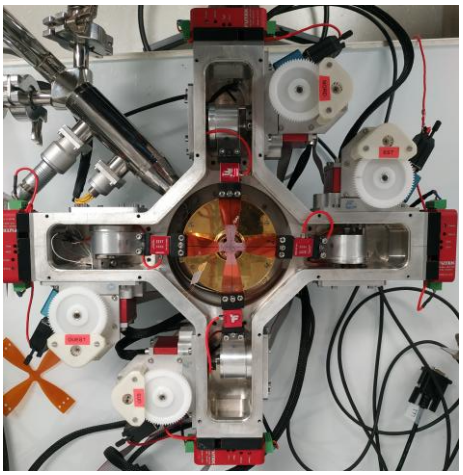

Figure 2: Cryogenic biaxial tensile stress device

The present results confirm the existence of an orientational transition of the charge density wave from ***c*** to ***a*** in GdTe3 during the deformation of the material along ***a*** axis at room temperature. This tends to confirm the general nature of this property in the RTe3 family having already been observed in TbTe3 [2].

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Slave Spin Mean Field theory in phases without and with broken symmetry

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This work explores how electrons behave in materials where strong interactions can change the phase of the system. Using the Slave Spin Mean Field Theory (SSMFT), we study the two-dimensional Hubbard model to understand phases with and without broken symmetry.

In the paramagnetic phase, we examine how increasing the interaction strength drives the Mott metal–insulator transition, where electrons change from being mobile to localized. We also study the effect of doping, which moves the system away from half-filling and influences the occurrence of the Mott transition. In addition, we investigate how introducing next nearest neighbor hopping (t') creates frustration, making stronger interactions necessary for the system to become insulating.
In the antiferromagnetic phase, where neighboring electrons align in opposite directions via slater mechanism at weak coupling, we explore how doping and frustration reduce magnetic order.

Overall, our study highlights how doping, lattice geometry and frustration affect the onset and stability of Mott insulating and antiferromagnetic phases within the slave spin framework, providing insight into the interplay between electron correlations and magnetic ordering.

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Pressure-temperature dependence of monoclinicity in a pseudo-tetragonal lattice of $La_4Ni_3O_{10+\delta}$

S. Ramakrishnan*[1], Y. Gao [1], E. Pachoud [1], G. Garbarino [2], M-A. Méasson[1], P. Toulemonde[1] and P. Rodière[1]

At ambient conditions the tri-layer superconducting nickelate $La_4Ni_3O_{10}$ possesses a monoclinic structure described by the space group $P2_1/a$. The compound is reported to undergo two structural transitions where it becomes tetragonal *I4/mmm* around 1000 K [1] and the other at 130 K [2], where the latter is proposed to be a density wave (DW) ordering. Presently, from high quality single crystals synthesized by flux it is realized that the monoclinic distortion is negligible and the structure is a derivative of the I4/mmm crystal structure. The tetragonal-to-monoclinic transition is characterized by the appearance of superlattice reflections at commensurate positions q = (½, ½ , 0) on an I-centered lattice. This can be suppressed down to 20 K from 1000 K at 14 GPa, prior entering the superconducting state. Incommensurate satellite reflections associated with the DW ordering remain undetected down to 20 K at ambient pressures. However, new phonon modes due to minute distortions are observed from Raman spectroscopy below 130 K presumably due to its high sensitivity compared to x-rays, where the degree of distortions are possibly controlled by the oxygen level in the sample.

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Inelastic neutron scattering study of magnon band structure in the kagome magnet $HoMn_6Sn_6$

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Magnetic kagome layers crystals consisting of corner sharing triangles have been found to possess various topological electronics properties such as giant anomalous Hall effect [1] or nodal points (e.g. Dirac point) in the band structure. Especially, the RMn_6Sn_6 (where R is a rare earth-Ho, Tb, Y, Tb, Lu...) family has gained recent interest precisely due to the presence of two Mn-based kagome planes. Additionnaly, the R-site plays an important role in the magnetic order of the system [2] and has consequent impact onto the topological electronic band structure. In addition to fermionic topology, topological magnons are also expected in this class of material and have been experimentally reported in YMn_6Sn_6 [3]. In our work, we choose to study specifically $HoMn_6Sn_6$. Because of antiferromagnetic Mn-Ho magnetic couplings, this compound exhibits a spin reorientation below a temperature T_{SR} = 220 K, characterized by a transition from a ferromagnetic (FM) state where the spins lie in the basal (*a*, *b*) plane to a FM state where the magnetics moments are partially aligned along the *c*-axis [4]. We recently performed a neutron scattering study on this compound to determine the evolution of the magnetic structure and the associated low energy magnonic band structure to better understand this spin-reorientation transition and the competing terms into the Hamiltonian. This preliminary study will pave the way to future studies at higher energies to probe potential topological magnonic features.

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Raman spectroscopy of $ErTe_3$ under anistropic strain

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Quantum materials or systems with strong electronic correlations exhibit multiple complex electronic orders, which are generally in competition with each other, such as superconductivity, magnetism and charge orders. Rare earth tritellurides RTe3 (with R=Y, La-Nd, Sm, Gd-Tm) with an orthorhombic structure are paradigmatic charge density wave (CDW) compounds with one or two quasi-degenerate 1Q CDW orders with orthogonal orientations [1]. The direction of the 1Q-CDW modulation is dictated by a weak structural anisotropy associated with a slip plane [2].
Here I will present Raman spectroscopy measurements coupled with a uniaxial strain device performed on the ErTe3 compound. I will show that the anisotropy of the CDW amplitude mode observed in Raman can be used to determine the orientation of the CDW order. I will then highlight the controlled reversal of the CDW orientation by uniaxial strain. Finally, I will discuss the unexpected presence of a unique monoclinic distortion in the 1Q-CDW state, suggesting a more complex order than initially anticipated.

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Relationship Between Nanostructure and Electrical Transport in HTS Superconductors Under High Magnetic Fields

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High-temperature superconductors (HTS) are key candidates for next-generation high-field magnets, with potential breakthroughs in medical imaging, nuclear fusion, and compact energy technologies. Their performance is determined by the critical current Ic, governed by vortex pinning efficiency. While I_c has been extensively studied at moderate fields, its behavior under extreme conditions (>30 T) remains largely unknown due to major experimental challenges. Yet, this regime is decisive for evaluating dissipation limits and unlocking disruptive applications.

In this work, conducted during a pre-doctoral internship at LNCMI-Toulouse, we contributed to the qualification of a unique experimental platform capable of measuring I_c in pulsed magnetic fields up to 60 T and temperatures ranging from 1.5 K to 77 K. The setup, among the very few worldwide, was benchmarked under static fields up to 12 T using a cryogen-free He^4 cryostat, demonstrating excellent reproducibility. First experiments in pulsed fields validate the robustness of the methodology and open unprecedented access to the high-field regime of HTS conductors.

Beyond its technological relevance, this work also provides a rare opportunity to address fundamental questions of vortex physics. Entering the 60 T regime allows one to probe vortex matter in an extreme density limit, where conventional pinning models may no longer apply. By mapping the field and temperature dependence of I_c, it becomes possible to test theoretical frameworks of collective versus strong pinning, explore the onset of flux-flow dissipation, and investigate the boundaries of the irreversible superconducting state. Importantly, these measurements offer direct benchmarks for theoretical and numerical models of vortex dynamics, enabling the community to validate simulations against experimental data in a regime previously inaccessible. Such experimental-theoretical dialogue is crucial to refine our microscopic understanding of high-temperature superconductivity.

$U_{13}Pd_{47}Ge_{25}$: a quasicrystalline Tsai-type approximant with spin-glass behaviour

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Since their discovery by Shechtman et al. in 1984 [1], quasicrystals and their approximants have attracted considerable scientific interest, not only for their exceptional crystallographic properties, but also for their wide range of chemical and physical properties and related applications [2].

The cubic YCd_6 structure-type and its derivatives form a well-known family of 1/1 Tsai-type quasicrystal approximants [3]. While many 4f element-based intermetallics belong to this family, examples with actinides are much scarcer, with only $NpCd_6$ and $PuCd_6$ appearing in databases. We recently discovered the formation of the ternary $U_{13}Pd_{47}Ge_{25}$ phase [4] adopting this structure type. Examination of the crystal structure by X-ray and electron diffractions confirms the presence of a pseudo-5-axis originating from the stacking of endohedral clusters.

The crystallographic details of this germanide (i.e. triangular network of U1, large cage around U2, mixed occupancy of two Pd/Ge sites) are favourable for the occurrence of magnetic frustration. Consequently, spin-glass like features are evident in the magnetic properties, specific heat and electrical resistivity of this material. Furthermore, these physical properties are influenced by the crystallographic disorder.

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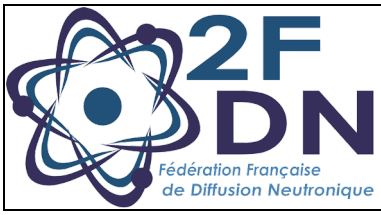	**2FDN** Fédération Française de Diffusion Neutronique
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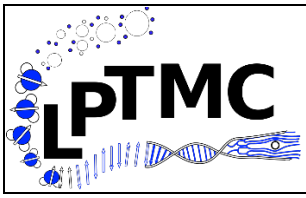	**LPTMC** Laboratoire de Physique Théorique de la Matière Condensée
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