Emergent Quantum States in Correlated Materials

Abstracts & Conference Handbook

Materials
Advances in Theory
Emergent properties

Superconductivity
Extreme conditions
Emergent magnetism

Organized by the GDR MEETICC

June 23-25,2025, Amphi Joliot-Curie, Paris-Saclay University

INSTITUT INTÉGRATIF DES MATÉRIAUX
université PARIS-SACLAY
FACULTÉ DES SCIENCES D'ORSAY
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Monday 23rd, june

13h00 – 13h30 : **Welcome coffee**

Session « Theoretical advances in Quantum Materials »

13h30 – 14h00 : **L. Reining** *(invited)*, "About the use of models to compute interaction effects"

14h00 – 14h20 : **B. Lenz**, "Universal Waterfall Feature in Cuprate Superconductors: Evidence of a Momentum-Driven Crossover"

14h20 – 14h40 : **L. Engstram**, "Upper critical field and pairing symmetry of Ising superconductors"

14h40 – 15h00 : **L. De' Medici**, "Paradigm for Finding d-Electron Heavy Fermions: The Case of Cr-doped CsFe2As2"

15h00 – 15h20 : **F. Cassol**, "The Optical conductivity of Ba2IrO4 and Sr2IrO4 : beyond the conventional interpretation of the double-peak structure"

15h20 – 16h00 : **Coffee break**

Session « Emergent magnetism»

16h00 – 16h30 : **P. McClarty** *(invited)*, "Altermagnetism: a perspective from symmetry"

16h30 – 16h50 : **Q. Meier**, "Altermagnetism from Orbital Ordering the Ruddelsden-Popper Chromates"

16h50 – 17h10 : **A. Devillez**, "Bond-dependent interactions and ill-ordered state in the honeycomb cobaltate BaCo2(AsO4)2"

17h10 – 17h30 : **F. Morineau**, "Satisfaction and Violation of the fluctuation-dissipation relation in spin ice"

17h30 – 17h50 : **Y. Oubaid**, "Interplay of Magnetism, Structure, and Electronic Properties in the Iron-Based Superconductor BaFe2S3"

18h00 – 20h00 : **Poster session and Diner cocktail**

Tuesday 24th, june

Session « Emergent properties I »

09h00 – 09h40 :	**P. Loubeyre** *(invited)*, "Quantum Effects in Highly Dense Hydrogen : Which measurements can be made and What insights can be gained ? "
09h40 – 10h00 :	**T. Desort**, "Quantized and nonquantized Hall response in topological Hatsugai-Kohmoto systems"
10h00 – 10h20 :	**C. Brun**, "Mott physics on a triangular lattice studied in two-dimensional surface supported materials"
10h20 – 10h40 :	**R. Tomar**, "Engineering a two-dimensional electron gas in BaTiO3 thin films: can ferroelectricity and metallicity coexist?"
10h40 – 11h10 :	**Coffee break**

Session « Extreme conditions I »

11h10 – 11h50 :	**F. Duc** *(invited)*, "Investigating new states of matter by neutron diffraction in high pulsed magnetic fields"
11h50 – 12h10 :	**D. Vignolles**, "Recent development of transport measurements in the Megagauss installation (beyond 101 T)"
12h10 – 12h30 :	**C. Ménil**, "Magnetic memory and hysteresis in ferromagnetic Weyl semi-metal Co3Sn2S2"
12h30 – 14h00 :	**Lunch break**

Session « Extreme conditions II »

14h00 – 14h40 :	**D. Carpentier** *(invited)*, "Topological semi-metals, anomalous electrodynamics and non-reciprocal optical response"
14h40 – 15h00 :	**A. Gallo--Frantz**, " Evidence of Fermi surface modification in NbSe3 under biaxial tensile stress "
15h00 – 15h20 :	**T. Vasina**, "Identicality of the High-Field and High-Pressure Superconducting Phases in UTe2"
15h20 – 15h50 :	**Coffee break**

Tuesday 24th, june

Session « Superconductivity »

15h50 – 16h30 : **A. Cano** *(invited)*, "Nickelate superconductors: emancipating from the cuprates"

16h00 – 16h30 : **A. Subedi**, "Pressure-tunable structural instabilities in single-layer-trilayer La3Ni2O7 "

16h30 – 16h50 : **P. Toulemonde**, "Pressure and temperature phase diagram of La3Ni2O7 nickelate"

16h50 – 17h10 : **D. Zhang**, "Democratizing nickelates superconductors: Topotactic reduction induced by aluminum sputter deposition"

17h10 – 17h30 : **C. Marrache**, "Pair-breaking in the granular quasi-one-dimensional organic superconductor (TMTSF)2ClO4"

19h00 – 23h00 : **Gala dinner**

L'Aquarelle Café
51 rue de Paris
91400 Orsay

Wednesday 25th, june

Session « Materials I »

09h00 – 09h40 :	**M. Saitta** *(invited)*, "Artificial Intelligence in Computational Materials Science: From the Origins of Life to Energy"
09h40 – 10h00 :	**M. Frachet**, "Colossal c-axis response and lack of rotational symmetry breaking within the kagome plane of the CsV3Sb5 superconductor"
10h00 – 10h20 :	**W. Liege**, "Search for orbital magnetism in the kagome metal CsV3Sb5"
10h20 – 10h40 :	**A. Favier**, "NMR local investigation of the spin liquid herbertsmithite: defects versus kagome physics"
10h40 – 11h10 :	**Coffee break**

Session « Emergent properties II »

11h10 – 11h50 :	**E. Collet** *(invited)*, "Propriétés émergentes : de l'équilibre à la dynamique ultrarapide"
11h50 – 12h10 :	**M-A. Measson**, "Multilayer Crystal Field states from locally broken centrosymmetry"
12h10 – 12h30 :	**L. Fratino**, "Voltage-controlled magnetism driven by electrical triggering of a metal-insulator transition"
12h30 – 12h50 :	**R. Nutakki**, "Deep translationally-symmetric neural quantum states for frustrated magnets"
12h50 – 14h00 :	**Lunch break**

Session « Materials II »

14h00 – 14h40 :	**N. Avarvari** *(invited)*, "Chirality related effects in molecular materials"

Oral contributions

Oral contributions

Poster contributions

About the use of models to compute interaction effects

Ayoub Aouina[1,2], Jaakko Koskelo[3,2], Matteo Gatti[2,3,4], and Lucia Reining*[2]

[1]Ruhr-Universität Bochum – Allemagne
[2]European Theoretical Spectroscopy Facility – Belgique
[3]Laboratoire des Solides Irradiés, Ecole Polytechnique – CNRS : UMR7642, CEA, Ecole Polytechnique – France
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The Coulomb interaction is responsible for many interesting properties of matter. The bare interaction is the same in every material, but its effects are not, and to predict or calculate these effects remains a challenge.
We will briefly discuss general strategies that are rely on functionals of quantities such as Green's functions, the one-body reduced density matrix, or the density. We will consider Density Functional Theory, Many-Body Perturbation Theory, and Dynamical Mean Field Theory on the same footing and investigate the difficulties of finding approximations. Models play a crucial role in this context, since they encode general knowledge about interaction effects.
In particular, we will discuss ways in which models make first principles electronic structure calculations feasible. This relies on powerful methods, including wavefunction-based ones, to provide benchmarks and solutions. While local models, such as the Anderson Impurity Model, are traditionally used to access strong correlation, here we will concentrate on another prominent model, the homogeneous electron gas, whose spectroscopic properties still have to be explored. We will discuss electron-hole correlation in the low-density regime (1), comparing to the more familiar excitonic effects in semiconductors and insulators. Finally, we will show how one may use models in a well defined and systematic way (2), in order to design new classes of functionals.

(1) J. Koskelo, L. Reining and M. Gatti, Phys. Rev. Lett. 134, 046402 (2025)
(2) M. Vanzini, A. Aouina, M. Panholzer, M. Gatti, and L. Reining, npj Comput Mater 8, 98 (2022)

Universal Waterfall Feature in Cuprate Superconductors: Evidence of a Momentum-Driven Crossover

Benjamin Bacq-Labreuil[1,2,3], Chafic Fawaz[4], Matteo D'astuto[4], Silke Biermann[1,5], and Benjamin Lenz*[6]

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[2]*Département de physique [Sherbrooke] – Canada*
[3]*Institut de Physique et Chimie des Matériaux de Strasbourg – université de Strasbourg – France*
[4]*Institut Néel – Centre National de la Recherche Scientifique, Université Grenoble Alpes, Institut polytechnique de Grenoble - Grenoble Institute of Technology, Centre National de la Recherche Scientifique : UPR2940, Institut Polytechnique de Grenoble - Grenoble Institute of Technology – France*
[5]*Collège de France – Collège de France – France*
[6]*Institut de minéralogie, de physique des matériaux et de cosmochimie – Sorbonne Université, Centre National de la Recherche Scientifique, Muséum National d'Histoire Naturelle (MNHN) – France*

We study two related universal anomalies of the spectral function of cuprates, so-called waterfall and high-energy kink features, by a combined cellular dynamical mean-field theory and angle-resolved photoemission study for the oxychloride NaxCa2–xCuO2Cl2 (Na-CCOC) (1). Tracing their origin back to an interplay of spin-polaron and local correlation effects both in undoped and hole-doped (Na-)CCOC, we establish them as a universal crossover between regions differing in the momentum dependence of the coupling and not necessarily in the related quasiparticles' energies. The proposed scenario extends to doping levels coinciding with the cuprate's superconducting dome and motivates further investigations of the fate of spin polarons in the superconducting phase.

(1) B. Bacq-Labreuil et al., Phys. Rev. Lett.134, 016502 (2025)

Upper critical field and pairing symmetry of Ising superconductors

Lena Engström*[1], Ludovica Zullo[2], Tristan Cren[3], Andrej Mesaros[1], and Pascal Simon[1]

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[2]*Universität Würzburg – Allemagne*
[3]*Institut des Nanosciences de Paris – Sorbonne Universite, Centre National de la Recherche Scientifique, Centre National de la Recherche Scientifique : UMR7588 – France*

Several conflicting predictions have been made for the symmetry of the pairing in transition metal dichalcogenide (TMD) superconductors. An indication of if singlet or triplet pairing is present can be given by the upper critical field (Hc), the magnetic field required to fully supress superconductivity. Monolayer NbSe2 and TaS2 have extremely large critical fields, due to a large Ising spin-orbit coupling (SOC) (1), yet they do not scale with SOC and temperature as expected for other TMDs(2).
I will present our theoretical work (3), in which we highlight that the Ising SOC has nodal lines in the Brillouin zone imposed by symmetry. By deriving the susceptibility, we have found that the scaling of the critical field can be traced back to whether the Fermi surface intersects with these lines or not. Reinterpreting existing experimental data, we find that only a predominantly singlet order is consistent with the measured Hc for several superconducting TMDs. Our analysis, utilizing symmetry properties to examine the interplay between spin-orbit coupling and superconductivity under high magnetic fields, extends to other layered superconductors.

(1) Frigeri, P.A., et al., 2004, New J. Phys. 6 115
(2) de la Barrera, S.C., Sinko, M.R., Gopalan, D.P. et al., 2018, Nat Commun 9, 1427
(3) Engström, L., Zullo, L., Cren, T., Mesaros, A., & Simon, P., arXiv: 2504.20775

Paradigm for Finding d-Electron Heavy Fermions: The Case of Cr-doped CsFe2As2

Luca De' Medici*[1]

[1]*Laboratoire Léon Brillouin – Institut Rayonnement Matière de Saclay (DRF), Université Paris-Saclay, Centre National de la Recherche Scientifique – France*

We define a general strategy for finding new heavy-fermionic materials without rare-earth elements: doping a Hund metal with pronounced orbital-selective correlations towards half filling. We argue that in general band structures, a possible orbital-selective Mott transition is frustrated by interorbital hopping into heavy-fermion behavior - where d orbitals provide both the heavy and the light electrons - which is enhanced when approaching half-filling. This phase ultimately disappears due to magnetic correlations, as in a standard Doniach diagram. Experimentally we have hole doped CsFe2As2, a Hund metal with 0.5 electrons/Fe away from half-filling, and obtained a heavy fermionic state with the highest Sommerfeld coefficient for Fe pnictides to date (270 mJ/molK^2), before signatures of an antiferromagnetic phase set in.

Crispino et al., Phys. Rev. Lett. 134, 076504 (2025)

The Optical conductivity of Ba2IrO4 and Sr2IrO4 : beyond the conventional interpretation of the double-peak structure

Francesco Cassol*[1,2], L éo Gaspard[2,3], Cyril Martins[4], Michele Casula[2], and Benjamin Lenz[2]

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[3]LCPQ, Université Paul Sabatier - Toulouse III – Laboratoire de Chimie et Physique Quantiques (LCPQ), IRSAMC, UMR 5626 CNRS – France
[4]LPCQ, Université Paul Sabatier - Toulouse III – Université Paul Sabatier - Toulouse III : UMR5626 – France

Since the discovery of their exotic spin-orbital entangled insulating ground state, Ba2rO4 and Sr2IrO4 have attracted considerable attention. Motivated by their structural similarities to cuprate high-Tc superconductors, numerous studies have explored their magnetic and electronic properties. For both compounds, optical transport quantities-such as optical absorption and optical conductivity-are characterized by a peculiar double-peak structure. The lower-energy peak, **α**, and the higher-energy peak, **β**, are conventionally associated with intra-band and inter-orbital excitations, respectively.

In this work, we revisit this topic by investigating the optical transport properties of Ba2IrO4 and Sr2IrO4 using a combination of theoretical techniques, and we compare our simulations with experimental data previously reported in the literature.

We compute the optical conductivity for both compounds beyond the Peierls substitution scheme, within the framework of dynamical mean-field theory (DMFT) for correlated electrons. By explicitly including both j=1/2 and j=3/2 states in the DMFT self-consistency loop, we characterize the nature of the double-peak structure.

Our results show good agreement with earlier experimental findings for both materials. Notably, in the case of Sr2IrO4, we successfully capture the temperature dependence of the optical conductivity. Contrary to the traditional interpretation, we assign a mixed j character to both the **α** and **β** peaks.

Furthermore, by comparing our DMFT results with self-consistent Born approximation (SCBA) calculations performed on a simplified single-band j=1/2 model, we show that the characteristic double-peak structure in the conductivity originates from the presence of spin- polarons in the unoccupied part of the spectrum.

Altermagnetism: a perspective from symmetry

Paul Mcclarty*[1]

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Altermagnets are compensated magnets whose band structures exhibit a characteristic pattern of spin splitting in momentum space. In this talk, I explain the physics of altermagnets based on symmetry considerations. The effect is most cleanly defined in the zero spin-orbit coupling limit where a Landau theory can be formulated that captures some of the principal features including the spin splitting. The Landau theory also makes clear that there is a multipolar order at the heart of altermagnetism. Switching on spin-orbit brings new features that I shall describe. Time allowing, I shall outline ways to use neutron scattering to probe altermagnets.

Altermagnetism from Orbital Ordering the Ruddelsden-Popper Chromates

Quintin Meier*[1]

[1]Néel – Institut Néel, CNRS, Univ. Grenoble Alpes – France

The series of Ruddlesden-Popper chromates Srn+1 CrnO3n+1 is an exciting material class that show strong orbital ordering. In these materials, the Cr4+ ions exhibit an electronic configuration of (dxy)1(dxz/yz)1, in which the energy dxy orbital lowered due to the crystal field splitting in the layered geometry of the crystal structure. The doubly degenerate dxz/yz manifold shows a tendency toward orbital ordering driven by electronic interactions, resulting in a state where electrons occupy either the dxz or dyz orbital on neighboring chromium sites. This orbital ordering induces a metal-insulator transition in the low-n members of the series (1).

Using first-principles calculations, we explore the interaction between orbital ordering and antiferromagnetic order in these materials. We demonstrate that the translational symmetry breaking of the orbital ordering in these systems can maintain the non-relativistic spin splitting even in the absence of crystalline symmetry breaking. In the layered structures, the distinct orbital ordering and antiferromagnetic patterns can either align or anti-align in adjacent layers, resulting in altermagnetic or compensated (anti-)altermagnetic behavior. In the latter case, the altermagnetic spin splitting exhibits opposite signs in adjacent layers leading to globally to a globally non altermagnetic state, yet the layerwise spin splitting remains intact. The relative stability of the altermagnetic and anti-altermagnetic phases in these systems can be tuned through effective dimensionality and strain engineering.(2)

(1) S. Doyle, QNM et al, Phys. Rev. Materials 8, L071602 (2024)
(2) Q. N. Meier et al, arXiv:2502.01515

Bond-dependent interactions and ill-ordered state in the honeycomb cobaltate BaCo2(AsO4)2

Armand Devillez*[1], Julien Robert[1], Elsa Lhotel[1], Rafik Ballou[1], Charlotte Cavenel[1] Fabio Denis Romero[1], Quentin Faure[2], Henrik Jacobsen[3,4], Jakob Lass[3], Daniel Gabriel Mazzone[3], Ursula Bengaard Hansen[5], Mechthild Enderle[5], Stéphane Raymond[6], Sophie De Brion[1], Virginie Simonet[1], and Manila Songvilay[1]

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Following the proposed materialization of Kitaev-bond-dependent spin liquid physics in honeycomb lattices of heavy transition metals with 4d or 5d electrons (1), it has been proposed that this can be extended to 3d transition metals, in particular Co2+ (2). A first step in validating the prospect of finding a quantum spin liquid is to demonstrate the presence of these anisotropic bond-dependent interactions in such materials. These could promote new types of behavior or provide insight into certain materials not elucidated to date. This is the case of BaCo2(AsO4)2, a honeycomb cobaltate whose ground state and Hamiltonian have been debated for decades (3).

We have investigated the magnetic properties of a BaCo2(AsO4)2 single-crystal through neutron diffraction and inelastic scattering, as well as by very-low temperature magnetization and AC susceptibility measurements. The latter measurements, which reveal slow dynamics and non-equilibrium responses, are consistent with an original ill-ordered magnetic compound with intrinsic defects as proposed previously (4): collinear zig-zag ferromagnetic chains in a up-up-down-down arrangement interspersed with additional chains to agree with the propagation vector of 0.27 imposed by competing interactions.

To interpret these results, we propose an exchange model with bond-dependent anisotropic interactions for nearest neighbors and Heisenberg interactions up to the fourth neighbors. Monte Carlo simulations show that our model successfully reproduces key experimental observations: spin-wave dispersions, magnetization curves with a 1/3 magnetization plateau, and the complex collinear spin configuration. This highlights the potential of including these new ingredients (anisotropic interactions) in understanding long-standing puzzling behaviors and discovering exotic physics.

(1) A. Kitaev, Ann. Phys. 321, 2 (2006) ; G. Jackeli Phys. Rev. Lett. 102, (2009).; (2) H. Liu, Phys. Rev. B 97, 014407 (2018) ; R. Sano, Phys Rev B 97, 014408 (2018).; (3) L.-P. Regnault, J. Phys. Soc. Jpn. 52, 1 (1983) ; R. Zhong, Physical Review B 106, 165131 (2022) ; T. Halloran, PNAS 120, e2215509119 (2023) ; (4) L.-P. Regnault, Heliyon 4, e00507 (2018).

Satisfaction and Violation of the fluctuation-dissipation relation in spin ice

Félix Morineau*[1], Vadim Cathelin[1], Peter Holdsworth[2], Sean Giblin[3], Geeta Balakhrishnan[4], Kazuyuki Matsuhira[5], Carley Paulsen[1], and Elsa Lhotel[1]

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[3]*Cardiff University – Royaume-Uni*
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[5]*Kyushu Institute of Technology – Japon*

Amongst the exotic magnetic states which emerge from frustrated spin systems, spin ices have aroused strong interest. Their excitations being described as magnetic charges, the so-called magnetic monopoles, govern the system dynamics, which are characterized by strongly diverging relaxation times at very low temperatures. Understanding monopole dynamics in spin ices remains a central challenge of frustrated magnetism, and their out-of-equilibrium properties are still poorly understood.

Recently, we developed a new experimental setup, which probes these properties by measuring both the out-of-phase part of the susceptibility $\chi''(f)$ and the magnetic noise $S(f)$. This allows us to directly measure the fluctuation-dissipation relation (FDR) (1), which provides an unambiguous test for out-of-equilibrium behavior in non-equilibrium statistical mechanics.

Thanks to this setup we could access the dynamics of the spin ice compounds $Dy_2Ti_2O_7$ and $Ho_2Ti_2O_7$ down to 150 mK, and address both the equilibrium and out-of-equilibrium regimes. In the two systems, we show that the FDR is satisfied down to 400 mK across the entire measured frequency range (from 0.001 Hz to 105 Hz), indicating that local equilibrium is achieved. Below 400 mK, violations to the FDR develop as an excess of noise at frequencies below 0.1 Hz, while at higher frequencies, the FDR remains valid down to 150 mK. Such deviations indicate the presence of several timescales in the system, which may be the signature of the lifting of the degeneracy of the spin ice Pauling states due to dipolar interactions.

(1) F. Morineau et al., Phys. Rev. Lett. 134, 096702 (2025)

Interplay of Magnetism, Structure, and Electronic Properties in the Iron-Based Superconductor BaFe2S3

Yassine Oubaid*[1,2], Victor Balédent[3], Pascale Foury-Leylekian[3], and Pierre Fertey[2]

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Recently, a family of quasi-1D Fe-based spin ladders compounds with the formula BaFeX, where X represents a chalcogen (Se or S), exhibit superconducting properties under pressures exceeding 10 GPa, with critical temperatures of approximately 10 K or 26 K, depending on the chalcogen species (1). However, the intriguing properties of these compounds extend beyond superconductivity. At ambient pressure, they behave as Mott insulators and display exotic structural and magnetic phenomena, including multiferroicity near room temperature. As such, these materials encompass key characteristics of strongly correlated quantum systems.

Building on extensive investigations of BaFeSe, this work presents a comprehensive experimental study of BaFeS. A detailed examination of the structural, magnetic, and electronic properties of BaFeS as a function of temperature-and to some extent under pressure. This included X-ray diffraction, neutron diffraction, and synchrotron-based infrared spectroscopy.

Our study has uncovered novel phases featuring new atomic structures, a previously unreported structural transition (to a polar structure), and demonstrating that BaFeS hosts a combination of an exotic tilted stripe magnetic order, multiferroicity and small magnetoelasticity (2). These findings have allowed us to refine existing interpretations and establish critical connections between these fundamental parameters.

In particular, we have significantly revised the interpretation of various experimental observations reported in the literature, substantially enhancing our understanding of magnetoelastic coupling, electronic gap opening, and structural degrees of freedom.

(1) H. Takahashi et al. Nature Materials, (2015)
(2) Y. Oubaid, submitted to PRL (2024); preprint : arXiv:2503.10942.

Topological semi-metals, anomalous electrodynamics and non-reciprocal optical response

David Carpentier[1*]

[1]ENSL, CNRS, Laboratoire de Physique, F-69342 Lyon, France

I will introduce pedagogically the notion of relativistic semi-metals, a material characterized by the crossing of electronic bands close to the Fermi level. I will pay a special attention to the simplest such semi-metals, denoted Weyl materials. After discussing their topological properties, I will introduce the anomalous electrodynamics of such materials, and its associated magneto-electric effect. As an illustration of the consequences of these anomalous electrodynamics, I will discuss the non-reciprocal optical response of such materials, and its potential applications. I will relate this non-reciprocity to the losses through optical modes of a Weyl slab, whose asymmetric dispersion originates from the anomalous electrodynamics.

Quantized and nonquantized Hall response in topological Hatsugai-Kohmoto systems

Thibaut Desort*[1], Mark Goerbig[1], and Corentin Morice[1]

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The Hall conductivity of insulators is well-known to be quantized, including in interacting systems (1). The Hatsugai-Kohmoto (HK) interaction (2), a type of Hubbard model diagonal in reciprocal space, is now widely studied in the context of topology, owing to the fact that its eigenstates, eigenenergies and Green's functions can be computed exactly. Using the Kubo formula, it is possible to access the Hall conductivity which has, even in the presence of the HK interaction, been reported to be quantized because it coincides with a Chern number (3). In this work, using Zeeman fields, we lift the many-body degeneracy induced by the Hatsugai-Kohmoto interaction in the topological Kane-Mele model. This selects specific states within the ground-state manifold that reveal a surprising non-quantized Hall response.

(1) Q. Niu, D. J. Thouless, and Y.-S. Wu, Phys. Rev. B 31, 3372 (1985)
(2) Y. Hatsugai and M. Kohmoto, J. Phys. Soc. Jap. 61, 2056–2069 (1992) (3) P. Mai, B. E. Feldman, and P. W. Phillips, Phys. Rev. 5, 013162 (2023)

Mott physics on a triangular lattice studied in two-dimensional surface supported materials

Mohammadmehdi Torkzadeh[1], Cesare Tresca[2,3], Mathieu Lizée[1], François Debontridder[1], Marie Hervé[1], Giani Profeta , Tristan Cren[1], Matteo Calandra[1,4], and **Christophe Brun**[*1]

[1]*Institut des NanoSciences de Paris – CNRS Sorbonne Université, Sorbonne Université, CNRS : UMR7588 – France*
[2]*Università degli Studi dell'Aquila – Italie*
[3]*CNR (SPIN) – Italie*
[4]*Università di Trento – Italie*

2D materials are interesting for their reduced dimension and also because their interior is their own bulk. Surface sensitive probes are key for probing their local electronic or structural properties. In this spirit, finding 2D materials being Mott insulators in the undoped crystal structure, out of which unconventional superconductivity could emerge upon controlled doping, is exciting to revisit some of the key ingredients at play in high-temperature cuprates.
Here, I will focus on a class of 2D surface crystals not so well-known but enabling the kind of study mentioned above on a triangular lattice (1,2,3). I will present the combined experimental and theoretical results we have obtained on 1/3 monolayer of Sn and Pb grown on Si(111). Our studies show that this family of surface crystals offers a delicate interplay between charge, spin, and lattice degrees of freedom determining their precise groundstate (4,5,6,7). Finally, recent results suggest that indeed this class of 2D materials enables the emergence of unconventional superconductivity upon appropriate doping (8).

(1) G. Santoro et al. Phys. Rev. B 59, 1891 (1999)
(2) G. Profeta and E. Tosatti, Phys. Rev. Lett. 98, 086401 (2007)
(3) P. Hansmann et al., Phys. Rev. Lett. 110, 166401 (2013)
(4) C. Tresca et al. Phys. Rev. Lett. 120, 196402 (2018)
(5) C. Tresca et al. Phys. Rev. B 104, 045126 (2021)
(6) C. Tresca et al. Phys. Rev. B 104, 045126 (2023)
(7) M. Torkzadeh et al. in preparation (2025) (8) F. Ming et al. Nature Phys. 19, 500 (2023)

Engineering a two-dimensional electron gas in BaTiO3 thin films: can ferroelectricity and metallicity coexist?

Ruchi Tomar*[1], Benazir Fazlioglu-Yalcin[2], Anouk S Goossens[1], Thomas Buttiens[1], Elsa Gradauskaite[1], Luis M. Vicente-Arche[1], Lucia Iglesias[1], Roman Engel-Herbert[2,3], and Manuel Bibes[1]

[1]Laboratoire Albert Fert, CNRS, Thales, Université Paris-Saclay, 91767 Palaiseau, France
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The long-standing concept of ferroelectric metals, proposed by Anderson and Blount, challenges conventional wisdom by suggesting that ferroelectricity and metallic conductivity can coexist-despite the expectation that free carriers should screen electrostatic interactions essential for ferroelectricity.(1) This paradox was first experimentally addressed with discovery of ferroelectric-like distortions in metallic LiOsO3(2) and later in low-dimensional systems such as conducting WTe2.(3) An alternative strategy involves doping conventional ferroelectrics like BaTiO3(4) or Ca-substituted SrTiO3,(5) inducing metallicity while preserving structural transitions, though such materials lack switchable polarization. A recent approach overcomes this limitation by confining charge carriers at the surface of ferroelectrics, forming a two-dimensional electron gas (2DEG) while retaining an insulating and switchable ferroelectric bulk.(6)

Here, we report epitaxial growth of high-quality, single-domain ferroelectric BaTiO3 films on GdScO3 using pulsed laser deposition. These films exhibit excellent crystallinity, an elevated ferroelectric transition temperature, and remarkable endurance, showing no fatigue even after 1011 polarization switching cycles. We demonstrate that these films not only serve as robust templates for 2DEG generation but are also expected to exhibit tunable electronic properties governed by ferroelectric polarization of underlying BaTiO3, paving the way for novel device functionalities.

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Investigating new states of matter by neutron diffraction in high pulsed magnetic fields

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Over the past two decades, significant advances have been made in neutron diffraction in high magnetic fields, with experiments now pushing the limits to fields exceeding 40 T. This progress has been driven by the development of specialized pulsed-field devices, using short- or long-duration pulsed magnets (1-3). These advances surpass the limitations of current superconducting and resistive installations available at neutron sources, enabling the exploration of novel field-induced states. However, performing diffraction measurements in strong magnetic field environments remains a challenging task, requiring careful topic selection and expert preparation to ensure successful campaigns at neutron sources.

In this presentation, I will provide an overview of the 2 K/40-T pulsed field-cryomagnet, collaboratively developed by LNCMI-Toulouse, ILL-Grenoble, and CEA-Grenoble. This magnet has been in operation since 2015, serving the community on the triple-axis CRG-CEA spectrometer IN22 at the ILL. Through a selection of results, I will highlight the capabilities of this setup and discuss the technical challenges encountered. Moreover, I will outline the necessary improvements essential for routine studies of materials with small magnetic moments, such as high Tc superconductors or quantum spin systems.

(1) S. Yoshii et al., Phys. Rev. Lett. 103 (2009) 077203.
(2) F. Duc et al., Rev. Sci. Instrum. 89 (2018) 053905.
(3) E. Fogh et al., Phys. Rev. B 101 (2020) 024403.

Recent development of transport measurements in the Megagauss installation (beyond 101 T)

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High magnetic fields have proven instrumental in exploring the physical properties of condensed matter, leading to discoveries such as the quantum Hall effect in 2D heterostructures and quantum oscillations in cuprate superconductors. In this talk, we present the development of a microwave technique for performing two-point transport measurements in semi-destructive pulsed magnetic fields (up to 150 T) and at low temperatures (down to 1.5 K). This new setup was tested on a variety of samples, and we report preliminary results on the metal-insulator transition in InAs and the observation of quantum oscillations in WTe2. Notably, we present the first observation of Shubnikov-de-Haas oscillations at magnetic fields exceeding 101 T.

Magnetic memory and hysteresis in ferromagnetic Weyl semi-metal Co3Sn2S2

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CoSnS, a ferromagnetic Weyl semimetal with Co atoms on a Kagome lattice has generated much recent attention. From electronic properties, it serves as a platform for exploring Weyl fermion physics with broken time-reversal symmetry. From magnetic properties, experiments have identified a temperature scale below the Curie temperature, associated with a, still debated, secondary magnetic phase. After introducing key properties of CoSnS, I will present magnetization measurements that reveal a memory effect which can be erased by applying a large magnetic field. We attributed this effect to a small secondary spin population with a coercive field significantly larger than that of the majority spins. Additionally, the shape of magnetization hysteresis curves can be understood through a surprisingly simple model in which the demagnetizing field plays a crucial role in defining a threshold between two distinct hysteresis regimes. By combining the effects of demagnetizing fields and memory, our results imply that the temperature scale below the Curie temperature is not a thermodynamic phase transition, but a crossing point between metastable boundaries.

Quantum Effects in Highly Dense Hydrogen : Which measurements can be made and What insights can be gained ?

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Understanding the properties of hydrogen systems - atom, molecule, solid - has played a central role in the development of quantum physics. The prediction of an atomic metallic phase at extremely high pressure has motivated theoretical and experimental research since the 1930s.

In this presentation, we aim to provide a state-of-the-art overview of current research on ultra-dense hydrogen. What can we learn? What are the theoretical and experimental challenges? Could these properties be observed at ambient pressure?

(1) Synchrotron infrared spectroscopic evidence of the probable transition to metal hydrogen. P. Loubeyre, F. Occelli and P. Dumas. Nature 577, 631 (2020).
(2) Compression of D2 to 460 GPa and Isotopic Effects in the Path to Metal Hydrogen. P.Loubeyre, F. Occelli and R. LeToullec. Phys. Rev. Lett. 129, 035501 (2022).
(3) Enabling quantum sensing under extreme pressure: Nitrogen-vacancy magnetometry up to 130 GPa. A. Hilberer et al. Phys. Rev. B 107, L220102 (2023).

Evidence of Fermi surface modification in NbSe3 under biaxial tensile stress

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Charge Density Waves (CDW) have been drawing attention for decades due to their ubiquity in low-dimensional correlated systems as well as their non-linear electrical properties under electric-field. Their sensitivity to the host lattice, through the electron-phonon coupling, makes the application of strain a key to study this electronic phase and more generally, to explore the phase diagram of the compounds. We will present results obtained by biaxial mechanical deformation of the quasi-1D system NbSe3. This system is made of 3 types of chains and crystallizes in a monoclinic structure where chains are parallel to the b-axis. Due to the strong nesting conditions of the Fermi surface, NbSe3 displays two incommensurate CDWs at 145 K and 59 K respectively. The application of an electric field above threshold values, results in collective transport modes due to the motion of the incommensurate CDWs and called "sliding". The use of a cryogenic biaxial tensile device allowed us to deform the sample along the chains and perpendicularly and to probe the effect of the deformation on the lattice with XRD as well as the evolution of electronic properties with the 4-probe method. The results obtained are consistent with the literature and show a strong anisotropic mechanical behavior that can be correlated with the critical temperature variations. Finally, the evolution of the sliding of both CDWs under tensile stress suggests a modification of the Fermi surface curvature, consistent with the literature and with the variations of the lattice measured in XRD.

Identicality of the High-Field and High-Pressure Superconducting Phases in UTe2

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UTe2 is a novel unconventional heavy-fermion superconductor that gained a lot of attention in the last few years. One of its most striking features is the presence of multiple superconducting phases and the probable existence of spin-triplet superconductivity. Detecting phase transitions inside the superconducting regime requires the use of a thermodynamic probe. Ac calorimetry is a sensitive technique particularly suited for measurements in extreme conditions. Using this technique, in addition to the ambient pressure, low-field superconducting phase (SC1), two other superconducting phases were identified in previous works:

- A high-field phase (HF) induced by a strong magnetic field along the b-axis (1).
- A high-pressure phase (SC2) induced by hydrostatic pressure (2).

However, up to now, whether the HF and SC2 phases were connected, or two distinct phases was still an open question. To get a clear picture of the P-T-H phase diagram, we performed ac calorimetry under both pressure and high magnetic fields up to 30T.

Our calorimetry data unambiguously demonstrates that the HF phase continuously evolves into the SC2 phase when applying pressure. These results provide strong, thermodynamic proof that the order parameter of the pressure- and field-induced phases are one and the same, and thus that the mechanism underlying superconductivity in the SC2 phase of UTe2 may be stabilized by both pressure and field (3).

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(3) T. Vasina et al., Phys. Rev. Lett. 134, 096501 (2025).

Nickelate superconductors: emancipating from the cuprates

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The discovery of superconductivity in nickelate materials, first in thin films and more recently in bulk samples under pressure, represents one of the most significant breakthroughs in the field. In this talk, I will provide an overview covering both theoretical and experimental developments.

Pressure-tunable structural instabilities in single-layer-trilayer La3Ni2O7

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Layered nickelates are believed to exhibit superconductivity similar to that found in the cuprates. However, the precise crystal structure of the superconducting phase of the layered nickelates has not been fully clarified. I use first principles calculations to study the pressure dependence of the structural instabilities in the single-layer-trilayer La3Ni2O7, which is one member of the layered nickelates family that also shows signatures of superconductivity. I find a nearly dispersionless nondegenerate phonon branch in the parent P4/mmm phase that is unstable along the Brillouin zone edge M (12,12,0)
→A (12,12,12)
at all investigated pressures up to 30 GPa. Calculations show additional doubly-degenerate instabilities along the edge MA at lower pressures. I used group-theoretical analysis to identify the distinct low-symmetry distortions possible due to these instabilities and generated them using the eigenvectors of the unstable modes. Structural relaxations show that the lowest energy structures at 0 and 10 GPa involve condensation of both the nondegenerate and doubly-degenerate instabilities, which is in contrast to the experimental refinements that involve condensation of only the doubly-degenerate branch. I also find that structural distortions are energetically favorable at 20 GPa, contrary to the experiments that do not observe any distortions of the parent P4/mmm structure at high pressures.

Pressure – temperature phase diagram of La3Ni2O7 nickelate

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The discovery of unconventional superconductivity (SC) in thin film of hole-doped infinite-layer nickelate Nd1-xSrxNiO2 below Tc = 15-20K has suddenly refreshed the field of HTSC research. So far, no superconducting bulk nickelate was discovered until the recent report of SC near 80K in La3Ni2O7 (La-327) above a pressure P* = 14GPa. Instead of previous systems with NiO2 planes, La-327 contains apical oxygens connecting NiO2 planes through 3dz2 Ni orbitals which, under pressure, based on theoretical DFT calculations, contribute to supplementary pockets at the Fermi surface, in addition to the usual one derived from 3dx2–y2 orbitals, which seem essential for the occurrence of SC. Concomitantly at 300K a structural transition occurs from the initial Amam orthorhombic La-327 crystal structure to the Fmmm one, also orthorhombic, around 10-15GPa at 300K, accompanied by a change of the Ni-Oapical-Ni angle from 168◦ to 180◦, when solid or liquid pressure transmitting medium (PTM) is used. In this study, we revisit the P,T phase diagram, in particular in the low T range, using x-ray and neutron diffraction and helium, a better hydrostatic PTM than the ones used in previous studies. At 300K a phase transition from orthorhombic to I4/mmm tetragonal symmetry (i.e. not orthorhombic Fmmm symmetry) is found around P*~7.5GPa (i.e. at lower pressure than with other PTM). We were also able to follow this transition line down to 5K (and under pressure) where P* is increased to ~10GPa. This work establishes more precisely the localization of the tetragonal phase which is the right symmetry adopted in the superconducting state.

Democratizing nickelates superconductors: Topotactic reduction induced by aluminum sputter deposition

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The recent discovery of superconductivity in infinite-layer (IL) nickelates (ABO) has opened new avenues for understanding high-temperature superconductivity (1). IL nickelates are typically synthesized via topotactic reduction of the perovskite ABO phase using CaH as a reducing agent. However, synthesis remains challenging, and only a few groups can produce high-quality superconducting (SC) samples (2,3). Alternative approaches have been proposed, such as in-situ aluminum layer deposition by molecular beam epitaxy (3,4) or hydrogen gas bombardment (5,6), but these techniques are often difficult to access.
Here, we report a more accessible method to synthesize SC IL nickelate thin films of Pr0.8Sr0.2NiO2 using a sputtered aluminum overlayer as a reducing agent (8). By optimizing the Al deposition parameters, we achieved superconductivity via both in situ and ex situ reductions (after air exposure of the precursor ABO films). In situ Al reduction leads to improved film quality, reaching a maximum superconducting transition temperature Tconset of 17 K. This simplified approach enhances reproducibility and control over the topotactic process, providing a more accessible pathway for further exploration of superconductivity in nickelates.

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Pair-breaking in the granular quasi-one-dimensional organic superconductor (TMTSF)2ClO4

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In the quasi-one dimensional organic superconductor (TMTSF)2ClO4, the randomness of the non-centrosymmetric ClO4 anions, whose ordering dictates whether the system exhibits spin-density wave or superconducting phases, can be experimentally controlled via the rate at which the sample is cooled down across the anion order-disorder transition temperature TAO = 24 K (1). This compound therefore provides a rare opportunity to precisely study how non-s-wave superconductivity evolves with disorder.
In this study, we have measured the residual density of states in the low temperature limit, in order to determine the nature of the scattering channel. We have done so using electronic specific heat measurements on a unique (TMTSF)2ClO4 sample with a careful control of the non-magnetic defect concentration, so as to keep the amount of lone-pair electrons constant. We have shown that, at strong disorder, there is compelling evidence for the existence of Born (strong) scattering in this d-wave superconducting system. At low disorder, we have shown that scattering may very well be dominated by isolated impurities, possibly in the Unitarity limit (weak scattering). There then is a cross-over between the two scattering regimes controlled by the size of the anion-ordered domains, which, in turn, determines the elastic electron mean free path. Such a crossover presents an interesting path to control the effect of disorder in non-s-wave superconductors.

[1] For recent reviews, see: S. E. Brown, Physica C 514 (2015) 279; D. Jerome and C. Bourbonnais, C. R. Physique 25 (2024) 17
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Artificial Intelligence in Computational Materials Science: From the Origins of Life to Energy

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This seminar explores recent advances in AI-driven materials science, from prebiotic chemistry to state-of-the-art energy applications. Machine learning, thanks to algorithmic progress and ever-increasing computing power, is transforming both computational modeling and experimental characterization. As head of the CNRS research network "AI and Materials (IAMAT)," I will present how ab initio methods, advanced statistical tools, and AI-based techniques are being integrated to deepen our understanding of complex reaction networks and material behavior. We will highlight applications ranging from the modeling of molecular systems-such as novel pathways for biomolecule synthesis relevant to the origins of life-to the design of materials for energy storage, including supercapacitors and hydrogen storage systems. The talk will also cover how AI enhances atomistic simulations and improves experimental techniques like spectroscopy and imaging, illustrating the transformative role of artificial intelligence across the materials science landscape.

Colossal c-axis response and lack of rotational symmetry breaking within the kagome plane of the CsV3Sb5 superconductor

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Insulating kagome lattices have long been studied in the context of frustrated magnetism and the search for a spin liquid state. Nowadays, metallic kagome systems are attracting much attention, thanks to their rich band structure that features Dirac cones, van Hove singularities and flat electronic bands. Within the recently discovered AV3Sb5 (A=K, Rb, Cs) family, this rich band structure allows the development of a charge density wave and, importantly, superconductivity (1).
Electronic nematicity, the breaking of the crystal lattice rotational symmetry by an electronic degree of freedom, has been reported in CsV3Sb5 (2) and the fluctuations thereof suggested to be relevant to the cooper pairing (3). We investigate this possibility using electrical transport under anisotropic strain, specific-heat and thermal expansion measurements. Our results demonstrate that superconductivity and the charge ordered state are strongly competing, and that this competition is drastically influenced by c-axis pressure (4). Moreover, we report the lack of any evidence for an electronic nematic instability within the kagome plane, but instead of a large susceptibility to isotropic strain. In light of the previous studies, this strongly suggests that any breaking of the rotational symmetry is a consequence of the stacking of different C6-symmetric kagome planes along the c-axis.

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(2) Nie et al., Nature 604, 59-64 (2022)
(3) Sur et al., Nat. Comm. 14, 3899 (2023)
(4) Frachet et al., Phys. Rev. Lett. 132, 186001 (2024)

Search for orbital magnetism in the kagome metal CsV3Sb5

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Kagome metals of the AV3Sb5 types with A={K,Cs,Rb} are under the spotlight recently due to their strongly correlated electronic phases at low temperatures. For instance, CsV3Sb5 exhibits both a charge density wave order below 94K and a superconducting phase below 2.5K (B. R. Ortiz et al, Phys. Rev. Lett. 125, 247002, (2020)). These materials also show a strong anomalous Hall effect with no spin ordering found, both by muon spin spectroscopy and neutron diffraction. To explain this, a chiral flux phase, emerging alongside the charge density wave, has been theoretically proposed (S. Zhou and Z. Wang, Nat. Commun 13, 7288 (2022), X. Feng et al, Science Bulletin 66, 1384-1388, (2022)). Most models predict this phase to produce magnetic intensity at M1=(1/2 0 L) or M2=(1/2 1/2 L) reciprocal space positions with L={0,1/2} (2,3). After investigation, through polarized neutron diffraction experiments, we observed no signal at M1 ruling out the possibility of having a magnetic moment larger than 0.01 uB by vanadium atom. However, our measurements on M2 do not exclude the possibility of a magnetic signal with a moment lower than 0.03 uB by vanadium. This shows that flux models have to be refined, whether toward a lowering of the expected magnetic moment or toward a different flux pattern giving rise to magnetic intensity at other positions. This work was experimentally challenging and went close to the limit in precision obtainable with polarized neutrons in a reasonable measurement time (W. Liege et al, Phys. Rev. B 110, 19, 195109, (2024)).

NMR local investigation of the spin liquid herbertsmithite: defects versus kagome physics

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Spin liquids are an exotic class of matter where despite strong exchange interactions, no order arises. Beyond this simple view, more refined criteria for defining a quantum spin liquid (QSL) state have been proposed such as long-range entanglement and fractionalization of the excitations (spinons). In two dimensions, the most emblematic and apparently basic case of a kagome lattice with near neighbour Heisenberg antiferromagnetic interactions, remains an enduring theoretical problem. The pending questions address the class of spin liquid (U1 Dirac, Z2,...) that is actually realized.

The prime kagome QSL candidate, herbertsmithite ZnCu3(OH)6Cl2, has been extensively studied: the absence of order down to 10-4 J (J ~200K) was established via muon spin rotation and the expected continuum for fractional excitations has been observed through Inelastic Neutron Scattering. Recently a debate has settled about the influence on the ground state of defects, which are ubiquitous in all candidate materials.

I will present my PhD work which has focused on two main axes : (i) the study of a series of herbertsmithite powder samples with different, well-controlled Zinc composition x (ZnxCu(4x)(OH)6Cl2) through Cu NQR and magnetization, analysed by high temperature series expansion in collaboration with B. Bernu and L. Messio (LPTMC), aiming at characterizing the interaction between kagome and interlayer defect spins; (ii) the study of single crystals through 17O NMR experiments which provide a unique local perspective on the defect issue. Thus, our results single out the impact of defects on the susceptibility and dynamics of the kagome spins.

Emergent properties: from equilibrium to ultrafast dynamics

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Symmetry breaking plays a central role in the emergence of functional properties. Ferroic phases typically arise from a descending symmetry breaking, whereby a high-symmetry phase transitions to a lower-symmetry ordered phase. According to the laws of thermodynamics, low-entropy ordered phases tend to form at low temperatures, which limits the applicability of many materials. Although ascending symmetry breaking–where a lower-symmetry phase transitions to a high-temperature higher-symmetry one–has been reported in rare cases, the underlying driving forces often remain unclear.

Other instabilities, associated with changes in electronic states (such as charge transfer or spin state), also give rise to functional responses, which can be activated by light. In some materials, both aspects–isosymmetric electronic state conversion and ferroic ordering–are strongly coupled [1–6]. Their evolution can be described using Landau's theory of phase transitions.

Electronic bistability in functional materials constitutes a significant source of entropy gain, which can compensate for the entropic cost of symmetry breaking. This opens new perspectives for stabilizing ferroic functionalities at high temperatures or for inducing magnetoelectric effects. Likewise, in ultrafast photoinduced dynamics, the interplay between electronic bistability and symmetry change gives rise to complex nonequilibrium behaviors, ranging from the formation of small charge-transfer polarons to macroscopic phase transitions.

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(3) M. Hervé, Nature Commun. 15, 267 (2024)
(4) E. Collet, Advances in Physics: X 2161936 (2023)
(5) E. Dobbelaar, ACIE 67, e202114021 (2021)
(6) E. Collet, Physical Review Materials (2021)

Multilayer Crystal Field states from locally broken centrosymmetry

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Charge, spin, and orbital local degrees of freedom with intersite interactions are often- times sufficient to construct most quantum orders. This is conventionally true for f -electron systems, where the extent of the f -electrons and their associated crystal-electric-field (CEF) states are strongly localized. Here, polarized Raman spectroscopy measurements of a locally non-centrosymmetric compound, CeCoSi, unveil more CEF excitations than expected in the local model. We interpret this as experimental evidence for multilayer entangled CEF states, arising from the sublattice degree of freedom due to local centrosymmetry breaking. The sublattice combined with the CEF spin and orbital degrees of freedom provide an uncon- sidered means to form novel orders, not only in this system, but in any system exhibiting globally preserved yet locally broken centrosymmetry.

Voltage-controlled magnetism driven by electrical triggering of a metal-insulator transition

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Phase separation strongly influences magnetic and magnetotransport properties in correlated systems like rare-earth manganites. This talk shows how resistive switching in metal-insulator transition (MIT) materials enables electrically controlled phase separation.

MIT switching often forms spatial patterns (e.g., conducting filaments or insulating barriers), injecting distinct electronic/magnetic phases into homogeneous materials. In (La,Sr)MnO, a threshold voltage triggers an electrothermal MIT, creating a phase-separated state with a paramagnetic insulating barrier in a ferromagnetic metallic matrix (1). Magneto-optics confirms well-defined magnetic phases, while microdiffraction reveals inhomogeneous strain, suggesting a nonuniform temperature profile. Electrical control of these nonuniformities al- lows tuning magnetic properties, including voltage-triggered anisotropy switching (2) and magnetoresistance anomalies.

For added tunability, a CdS/LSMO heterostructure uses photocarrier injection to enhance LSMO conductivity (37% resistance drop at the transition temperature under light), comparable to a 9 T magnetic field. Surprisingly, optical and magnetic responses are decoupled (3).

These findings demonstrate voltage-controlled magnetism and highlight MIT materials as a nonlinear platform for studying magneto-thermal phenomena.

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Deep translationally-symmetric neural quantum states for frustrated magnets

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Many-parameter neural network quantum states combined with variational Monte Carlo have obtained state-of-the-art results for ground states of certain 2D frustrated quantum many-body spin systems. Successful architectures exploit translational symmetries, but there is no systematic understanding of the root of their success. Here, we apply a performant network from computer vision, which combines elements of different architectures, and through a series of numerical experiments distill the necessary ingredients to obtain accurate ground states. We then turn our attention to challenging 3D problems in frustrated magnetism, in particular the S = 1/2 Heisenberg model on the hyperkagome lattice, a minimal model for the iridate $Na_4Ir_3O_8$, where we discuss the difficulties in obtaining highly-accurate variational energies. This highlights the obstacles still to overcome in order to apply neural quantum states to a wider-range of models relevant to solid state experiments.

Chirality related effects in molecular materials

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Chiral electroactive materials (1) are gaining continuous interest in the frame of chirality related physical phenomena such as the electrical magnetochiral anisotropy (eMChA) effect or the chirality induced spin selectivity (CISS) effect. The eMChA effect expresses the dependence of the resistance of a chiral conductor on its handedness and on the relative orientation of the electrical current and the applied magnetic field,(2) whereas the CISS effect refers to the selective transmission of a preferential electron spin orientation through a chiral material.(3) Similarities and differences between the two effects have been recently discussed.(4) We will discuss evidences for the occurrence of the CISS effect in chiral tetrathiafulvalenes (TTF),(5,6) in thiadiazole-helicenes,(7) and in (6)helicene-bis(thiol) through single molecule break junction.(8) In the latter, the concomitant observation of the CISS and the eMChA effects was possible.

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Charge density waves in metallic / insulating phases of monolayer $TaSe_2$/GaP

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Transition Metal Dichalcogenides (TMDs) exhibit various electronic properties, including metallic, insulating, superconducting, and charge density wave (CDW) phases. Among the TMDs, 1T-TaSe2 displays a star-of-David CDW which induces an unusual strong correlation effect: an insulating surface layer while the bulk remains metallic (1). Monolayer 1T-TaSe has been shown to host a Mott insulating phase, which persists in few-layer systems but vanishes in thicker samples (2,3). In contrast, the 1H-TaSe phase remains metallic and superconducting at low temperatures, consistent with DFT predictions.

In 2016, Ma et al. (4) showed that STM voltage pulses could locally drive a transition from an insulating state with the famous star-of-David CDW to a metallic state with a mosaic CDW on the surface of bulk. This intriguing phenomenon can be useful for drawing electronic circuits on single atomic layer TMDs.

Thus, we have performed scanning tunneling microscopy/spectroscopy experiments to investigate electronic properties of monolayers of TaSe2 grown by Molecular Beam Epitaxy (MBE) on a GaP(111) surface. We are exploring samples consisting in mixed phases of 1T and 1H-TaSe2 domains covering approximately one monolayer, with few bilayer areas. Above the 1T-TaSe2 flakes, voltage pulses can be done in order to try to induce phase transitions from insulating to metallic state.

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Computing the one-body reduced density matrix with Quantum Monte Carlo for solids

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The one body reduced density matrix (1RDM) is a many-body object without a classical equivalent. It tells us a lot about the degree of correlation in the system, particularly how electrons occupy the single particle states (1). We have computed this object with Quantum Monte Carlo techniques for two systems. First, we have benchmarked the accuracy of QMC-1RDMs and densities, comparing them with the exact solution of the Helium atom, answering the question, 'Does a better QMC energy imply better observables? Most recently we have computed accurate RDMs for crystalline Silicon by treating the problem of finite system size. This now allows us to compute reliable RDMs for crystalline systems.

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Effect of Doping and Synthesis on the Structure and Magneto-electric properties of GaFeO3

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Gallium ferrite is a well-known single-phase multiferroic material. It has an orthorhombic structure in ambient conditions. It is attractive for applications due to its tunable physical properties with size, synthesis conditions, and Ga:Fe ratio (1). The high-pressure synthesis of GFO up to 70 GPa showed a sequence of phase transitions where the orthorhombic phase Pc21n changes to orthorhombic Pbnm and rhombohedral R3c (2). The low magnetic transition temperature (TC) and high leakage current are two drawbacks that hinder its practical applications. This study presents the effect of hydrothermal synthesis and Na doping on the structure and magneto-electric properties of GFO. The Rietveld refinement on PXRD data confirmed that Ga1-xNaxFeO3 crystallizes in a trigonal structure space group. Temperature-dependent magnetization revealed weak ferrimagnetism at room temperature, and there is a noticeable change in magnetization with Na doping, exhibiting a Morin-like (AFM) transition. The RT magneto-electric coupling coefficient and dielectric constant are enhanced compared to reported GFO at 4.2 K (1).

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Electronic and crystal structures of non-centrosymmetric EuTGe3 (T=Co, Rh & Ir) under high-pressure

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Intermetallic compounds EuT Ge (T = transition metal) crystallize in a non-centrosymmetric BaNiSn-type structure and have attracted considerable attention due to their complex magnetic ordering and pressure-induced phase diagrams that may accommodate superconductivity (1,2). At ambient pressure, divalent Eu ions (Eu2, 4f, J = 7/2) exhibit antiferromagnetic ordering below 15 K, with the magnetic ordering direction depending sensitively on the transition metal T (1).
In this work, we systematically investigated the pressure evolution of the electronic and crystal structures of EuTGe (T = Co, Rh, Ir) using high-resolution X-ray absorption spectroscopy and powder X-ray diffraction.
Our results reveal that the rate of Eu valence change under pressure varies depending on T. A continuous lattice contraction with increasing pressure was observed for EuCoGe (3), EuRhGe (4), and EuIrGe.
These findings provide new insight into the interplay between electronic structure, lattice symmetry, and emergent quantum phases in non-centrosymmetric Eu-based intermetallics.

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High pressure studies in pulsed magnetic field

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Pressure is a powerful tuning parameter for strongly correlated electron systems, especially in association with the other extreme conditions of low temperature and high magnetic fields. Combining high pressure with static magnetic field is quite common, even up to the highest static magnetic fields available in dedicated facilities. But if even higher magnetic field is required, only pulsed magnetic fields are available, and combing high pressure techniques with pulsed fields presents specific challenges, especially if low temperatures are required. In a collaboration between CEA Grenoble, CNRS LNCMI Toulouse, and Niigata university, we developed a pressure cell to perform magneto-transport measurements under pressure up to 6 GPa, in pulsed magnetic fields up to 60T and at temperatures down to 1.4K(1). We present the performance of the technique with some examples of studies in the systems CeRh2Si2(2), URu2Si2(3) and UTe2(4).

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Investigating Nanoscale Conducting Filaments in (V0.95Cr0.05)2O3 Mott Insulator for Resistive Switching Applications at Room Temperature Using In-Operando s-SNOM

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Nowadays, both volatile and non-volatile resistive switching induced by electric pulses are investigated, targeting resistive random-access memories and emerging technologies, such as neuromorphic computing and optoelectronic devices. In many oxides, resistive switching can be driven by the formation of conductive filaments the IMT is triggered by strong electric fields, which promote the electro-diffusion of either cations from the electrodes or oxygen vacancies in the oxide. However, in strongly correlated materials such as Mott insulators, including chalcogenides, vanadates, and rare-earth nickelates, the insulator-to-metal transition (IMT) is governed by a local Mott electronic phase transition: the electric Mott transition. 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. By using in operando scattering type-Scanning Near-field Optical Microscopy (s-SNOM), we investigated optical properties of (V0.95Cr0.05)2O3 polycrystalline thin films at nanoscale and controlled the non-volatile switching at room temperature. 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. We found that the infrared properties within the filament are very similar to those obtained under pressure from far-field optical spectroscopy on a (V0.95Cr0.05)2O3 single crystal.

La3Ni2O7–δ thin films under compressive strain

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Here, I will show our efforts to stabilize the RP LNO327 phase using the O2 partial pressure as knob during pulsed laser deposition. Thin films are grown onto LaAlO3 substrates by ablating a nominally stoichiometric LNO327 target. Progressively decreasing the Oxygen pressure, allows us to pass from the simple perovskite LNO113 at high pressure to the RP LNO327 phase at lower pressure, as attested via X-ray diffraction measurements. The fully metallic behavior of the LNO113 phase characterized also by very low resistivity values, was found to change towards a bad-metal behavior for the LNO327-phase exhibiting a slight upturn at low T and an overall larger resistivity. The further post-growth O2 annealing at high temperature resulted in no measurable effects on the transport properties of our LNO327 thin films. This suggests the key role played by the O3 post-annealing to get superconducting signatures in LNO327 thin films. I will also show the effect of different compressive strain states as induced by growth onto SrLaAlO4 and YAlO3 substrates on both structure and transport properties of LNO327 films.

Magnetic properties of the frustrated centered pyrochlore (Mn(II)(ta)2) studied by 1H-NMR

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Geometrical frustration in magnetic materials has proven to be extraordinary fertile ground for the discovery of new concepts and exotic quantum states of matter. Studies of materials with frustrated geometries such as the triangular, kagome, hyperkagome, or pyrochlore lattices have yielded a host of topical disordered and ordered states, among them spin ice, spin liquid, and spin glass states, for example. More recently, a new frustrated geometry has been discovered via molecular design of the metal-azolate framework (Mn(II)(ta)2), which realizes a closely related centered pyrochlore lattice of Mn spins with S = 5/2 (1). Theoretical work highlighted the rich phase diagram of the classical Heisenberg antiferromagnetic J1-J2 model, relevant for such compound, including partial ordering and highly degenerate spin liquid.
Here we present a first NMR study of (Mn(II)(ta)2), from the paramagnetic to the correlated spin-liquid regime down to 1.8K. Focusing on the 1H-NMR probe, we extract the temperature dependence of the local magnetic susceptibility and of the spin-lattice relaxation time T1. We will discuss our results in the light of the recent theoretical work obtained by classical Monte-Carlo simulations (2).

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Metastability of the Topological Magnetic Orders in the Chiral Antiferromagnet EuPtSi

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Over the past decade, topological properties have emerged as a central theme in condensed matter physics, influencing systems such as 2D electron gases in the quantum Hall regime, topological insulators, Weyl and Dirac semimetals, and topological superconductors. Interest has also grown in topological spin textures, particularly magnetic skyrmions-noncollinear spin configurations with topologically protected, particle-like states. Their stability at nanoscale sizes makes them promising candidates for future data storage technologies like racetrack memory devices. Typically, skyrmions observed in experiments behave as classical objects forming skyrmion lattices (SkL). However, the discovery of nanometer-sized skyrmions at low temperatures, where quantum effects are significant, has introduced the concept of quantum skyrmions, showing phenomena like quantum tunneling and energy level quantization. Recently, metastable skyrmion states have been observed in the SkL A-phase of the chiral antiferromagnet EuPtSi via field cooling. EuPtSi crystallizes in a non-centrosymmetric cubic chiral structure, forming a trillium lattice of corner-sharing triangles. This geometry results in strong magnetic frustration and gives rise to various topological magnetic phases below the Néel temperature (TN = 4.05 K), depending on the magnetic field orientation.We present a detailed investigation of the field-induced magnetic phases in EuPtSi using resistivity and Hall effect measurements at low temperatures. Our results confirm the metastable A-phase skyrmion state for H –– (111) and reveal similar metastability in the A and B phases for H –– (100), suggesting strong parallels among these phases, despite the lack of microscopic evidence for SkL presence in A and B.

Multiple magnetic transitions and coordination environments in the MCuFe2O5 (M = Mn and Co) high pressure oxides.

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Charge disproportionation has been revealed among the Fe ions in CaFe3O5, leading to the formula CaFe2+Fe23+O ((i)) 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 ((ii)) with a variety of magnetic order states below TN = 350 K (Mn) and 300 K (Co) ((iii),(iv)). Combining these ideas: i) substituting Fe2+ by Cu2+ and ii) Ca by Mn or Co via HPHT synthesis in CaFe3O5, we have obtained the novel M CuFe2O5 (M = Mn and Co) oxides at 10 and 20 GPa and 1273 K with a Walker-type multianvil press. Intriguingly, MnCuFe2O5 shows a different structure than CaCuFe2O5 and MnFe3O5 (Cmcm) and crystallizes in the Pnma space group. Contrarily, CoCuFe2O5 preserves the Cmcm structure. The thermal evolution of the magnetic susceptibility for CoCuFe2O5 (MnCuFe2O5) shows a sharp maximum at TN1 = 195 (105) K and a second transition at TN2 = 77 (39) K. It follows a Curie-Weiss behaviour above 300 (150) K and presents a – theta– = 700 (218) K with a μeff = 5.7 (6.6) μB/f.u, larger than the expected value of μtheo = 4.7 (5.2) μB/f.u. The field-dependent magnetization at 2 K of both systems indicates a ferrimagnetic arrangement. The detailed analysis will be presented.

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NMR study of a quantum spin liquid candidate: the triangular system $YbZn_2GaO_5$ with Jeff = 1/2

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The **Quantum Spin Liquid (QSL)** is an exotic state of matter that has intrigued both theorists and experimentalists for decades. It was first theoretically proposed by Anderson in 1973, who considered a frustrated triangular lattice of spin-1/2 moments interacting via antiferromagnetic exchange. The predicted unconventional ground state, emerging from the high temperature paramagnetic state without any phase transition is characterized by the presence of fractionalized excitations.
Since then, significant efforts have been devoted to realizing a material that could host such a state. In this study, we investigate the rare-earth-based compound **YbZnGaO**, in which the magnetic layers form a triangular lattice of **Yb^3** ions. The crystal electric field lifts the degeneracy of the Yb^3 electronic levels, resulting in an effective spin-1/2 ground state below approximately 400 K. The geometric frustration in this system is further enhanced by next nearest-neighbor exchange interactions, making it a promising QSL candidate (1).
Our investigation relies on **1/Ga NMR** measurements to explore both the spectral and dynamical properties down to helium temperatures. The spectral analysis provides insight into the evolution of internal magnetic fields and the local ionic environment-particularly addressing the crucial issue of disorder-while the dynamical measurements allow us to probe magnetic excitations and search for signatures of exotic power-law behaviors.

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Overcoming the limitations of SIMS technique for oxide chemical analysis

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Conventional post-growth techniques like diffractions and microscopies struggle for direct observations of light elements like oxygen or hydrogen, especially for thin films whose little amount of matter is a limitation. SIMS is a unique technique for in-depth chemical composition analyses. SIMS is well-known to have a great sensitivity for traces and it offers as well very high mass resolutions and enough depth resolution to study thin films.
The main limitation of SIMS comes from the impossibility to make quantitative measurements due to the matrix effect. Indeed, the secondary ion intensity results from the strongly out of equilibrium chemical reactions induced under the primary beam irradiation and occurring within a tiny space at a very high effective temperature. The strategy toward quantitative SIMS analysis of oxides not only relies on the phenomenological observation of standards but also includes the understanding of the major trends driving the matrix effect in a given family of compounds.
We report a systematic study of powders of nickelates Nd(1-x)CaxNiO3-d with x = 0.1, 0.2 and d = 0, 1. Their structures were determined with enough control to be used as references for SIMS analysis. Several experimental configurations were compared and we identified the most suited for oxygen analysis. Semi-quantitative measurements of the oxygen stoichiometry were achieved and the major factors driving the oxygen ionic intensity in several experimental configurations are discussed. The different origins of hydrogen content could be discriminated and the amount of hydrogenation induced by CaH2 and CaD2 reduction steps could be measured.

Phase Diagram of Pure and Cr-Doped VO under Temperature and Pressure: An Infrared Spectroscopy Study

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Vanadium sesquioxide (VO) is a prototypical strongly correlated electron system, well known for its Mott-Hubard metal-insulator transition. We explored the temperature–pressure phase diagram of pure and 5% Cr-doped VO between 300 K and 22 K and up to 14 GPa using infrared spectroscopy in a membrane-driven diamond anvil cell, enabling a simultaneous precise and independent control of pressure and temperature. In contrast to chemical doping, pressure allows exploration of the phase diagram without introducing additional chemical disorder. We analyzed the transitions between the paramagnetic insulating (PI), paramagnetic metallic (PM), and antiferromagnetic insulating (AFI) phases. In the pure compound the AFI–PM transition is abrupt, while in the doped sample it appears to be continuous. Analysis of the infrared spectra using an effective medium model reveals phase separation over a surprisingly broad pressure range, in agreement with complementary X-ray diffraction measurements under pressure. These results highlight the influence of chemical substitution and thus of disorder-on the nature of the AFI–PM phase transition.

Specific study of unconventional superconductor UCoGe

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The coexistence of ferromagnetism and superconductivity in the uranium compound UCoGe raises some fundamental questions about the nature of the pairing mechanism in this material 1. Here we report results of a specific heat study on a high quality UCoGe sample (RRR=200). Specific heat allows to follow the evolution of both the superconducting and the Curie temperature under field. By contrast with resistivity measurements, it has the advantage, for the superconducting transition, to yield a "bulk" value for the transition temperature which is not influenced by small (filamentary) regions of the sample which may be superconducting at higher temperatures in low field. The upper critical field of UCoGe has an anomalous behaviour for field applied along the b-axis, suggesting a field-reinforcement of the pairing 2,3. These measurements give a new support to this hypothesis, through the anomalous evolution of the specific heat jump along the Hc2 line. They will be contrasted with the behaviour observed in UTe2, which also show field-reinforced pairing. Measurements show a very strong dependence of the upper critical field HC2 with the field orientation. For H//c, HC2 remains very low whereas for H//b, the superconducting phase could be followed up to 15T. This anisotropy is another indicator of a field-dependant pairing mechanism. This result combined with previous studies suggest that longitudinal ferromagnetic fluctuations tuned by a magnetic field are the pairing mechanism responsible for the superconductivity in UCoGe4,5.

The 3D analogue of the Shastry-Sutherland model

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The Shasrty-Sutherland lattice, a paradigmatic model in frustrated magnetism, has been the source of exciting physics in the past decades, from experimental measurements of magnetisation plateaus to theoretical evidence of spin liquids. We propose here a 3D analogue of the 2D lattice, which can be seen as a J1–J2 deformed pyrochlore lattice where the coordination of each site is conserved but the topology is modified. We study the ground states of the model analytically in the classical Ising and Heisenberg regime, where we determine the exact ground states with respect to J2/J1 and an external field h. In the quantum Heisenberg regime we find a singlet state as the exact solution in the range $J2 \geq 2J1$, similarly to the 2D model, making this a rare example of a 3D quantum system where the exact ground state is known. We continue our analysis numerically for $J2 < 2J1$ using Exact Diagonalisation and Neural Quantum States where we will discuss differences in the phase diagrams of the 2D and 3D models.

Thermoelectric power in the unconventional superconductor CeRh2As2

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CeRh2As2 is an unconventional superconductor (Tc≈0.35K) showing two distinct superconducting phases when a magnetic field is applied along the crystallographic c-axis (1). This exceptional transition from a possibly low-field even-parity to a high-field odd-parity superconducting phase is explained by the lack of local inversion symmetry on the Ce site in the crystal structure. The transition between the two superconducting phases occurs at a field of about 4T for H//c and superconductivity persists up to Hc2=16T, in clear violation of the Pauli limit. Turning the magnetic field 30◦ from c-axis suppresses the high-field superconducting phase and Hc2 for H//a is about 2T (2). The normal state of CeRh2As2 is also highly anisotropic and shows two phases as a function of magnetic field, with a clear transition at Hcr ˜9T for H//a. The microscopic origin of these two phases and their possible feedback on the superconductivity is still under debate (3,4).
Here, we present measurements of the thermoelectric power S(T,H) of CeRh2As2 at different angles between the a and the c-axis. The thermoelectric power shows clear signatures of the different normal state phases. The absolute value of S/T becomes huge (˜25 μV/K2) around the Hcr transition line indicating strong electronic correlations. Furthermore, the Seebeck coefficient changes sign at Hcr which might point to a restructuration of the Fermi surface.

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Search of magnetic textures in high critical temperature superconducting cuprates

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The electronic phase diagram of high-Tc cuprates is dominated by a mysterious pseudo-gap (PG) phase, characterized by a partial gapping of the Fermi surface. Polarized neutron diffraction measurements have shown that the PG state of four different cuprate families contains a magnetic phase that breaks the inversion and time reversal symmetries. This phase has been interpreted as the signature of a loop-current magneto-electric quantum state [1, 2]. Since it preserves the translational symmetry of the lattice, it is referred to as "q=0 magnetism". The recent discovery of additional magnetic correlations induced by these quantum states within the CuO_2 planes of YBa2Cu3O6+**δ** and leading to a doubling of the unit cell (magnetism at q = 1/2) suggests the existence of a magnetic texture that could play a key role in the physics of the PG [3-5].
This work focuses on investigating such magnetic textures in the single-layer bismuth cuprate Bi2(Sr,La)2CuO6+**δ**, a system where neither of the q = 0 or q = 1/2 magnetisms have been explored so far. To enable this study, we are growing large single crystals with, various La content, using the crucible-free floating zone technique, which ensures high chemical and crystalline quality of the grown samples. These crystals will be examined using polarized neutron diffraction to search for the magnetic phases previously observed at q = 0 and q = 1/2 in related cuprate systems.

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Topology in correlated bands in generalised Hatsugai-Kohmoto models

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Topological properties of correlated systems have recently been studied in the presence of the Hatsugai-Kohmoto (HK) interaction, a Hubbard-like term diagonal in reciprocal space rather than in real space (1,2). This interaction was also generalised in the context of cuprate superconductors to finite momentum, yielding electronic structures strikingly close to that of the pseudogap phase (3). We study the influence of such a finite-momentum HK term on Haldane and Kane–Mele models, derive the Green's function and find complex connections between its poles and zeros as a function of reciprocal space and frequency, akin to the connected Fermi and Luttinger arcs discovered recently (3).

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Charge Modulation in the Vortex Halo of a Superconductor Enhances its Critical Magnetic Field

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When an orbital magnetic field suppresses superconductivity, forming periodic vortices in type-II superconductors, subdominant orders can emerge in the vortex cores. Rather than competing with superconductivity, we find that the emergent charge order within the halo of a vortex makes superconductivity more robust by enhancing the upper critical field. We establish that charge modulations nucleate in and around the vortex core for model parameters dictated by the underlying non-superconducting state. We further show that the spectral signatures from the Caroli-de Gennes-Matricon (CdGM) bound states in vortex cores track the charge modulation. The CdGM-like peak is found to shift toward the gap edge and oscillate from particle-to-hole bias from site to site, signaling charge modulation.

Absence of Pole–Zero Annihilation at the Edge of Topological Mott Insulators

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Green's function zeros (GFZs), which emerge in Mott insulators as signatures of electron fractionalization, have been proposed to carry topological significance and influence observable boundary phenomena. Recent studies suggest that GFZs can annihilate topological edge-state poles in interacting systems, implying a deep interplay between the two. However, conflicting results from different theoretical frameworks raise questions about the robustness of this annihilation. In this work, we revisit the interface between a topological Mott insula tor and a non-interacting topological insulator using two complementary approaches: the slave-rotor formalism and the Hubbard operator method. Our analysis shows that edge-state poles and zeros persist independently, and their annihilation does not occur. Our findings highlight the need for careful treatment of fractionalization effects in strongly correlated topological systems.

Flat bands and high-temperature superconductivity in Graphene

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It has been observed that ordered Erbium (Er) intercalation between single layer graphene and SiC(0001) results in an n-doped graphene superstructure with flat bands. This system provides a playground to study the interaction between magnetism, a divergent density of states at the Fermi level and superconductivity. Graphite intercalation compounds (GIC) have been studied for their potential to exhibit superconductivity (1). Inspired by this, graphene has been widely intercalated to engineer its electronic structure. Observations of intercalation involving graphene were obtained with noble metals like gold (2). Graphene has also been intercalated with a wide variety of atoms such as Li, K, Ca, Cs, and Rb (3). Lanthanide atoms provide higher levels of electron doping compared to alkali atoms. So Graphene was intercalated with Er-atoms (4). In this work, flatbands were observed in this Er- intercalated superstructure. Using Density Functional Theory, we study the effect of the intercalated Er superstructure on the electronic structure of monolayer graphene. We study the modification of the band structure and test the formation of flatbands, with the aim to evaluate the possibility of superconductivity in this and related structures.

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