Plenary Speakers

Radiation damage of high temperature superconductors for fusion magnets

Susan Speller¹

¹University of Oxford, United Kingdom

Plenary Speaker: Susan Speller, University of Oxford, UK, June 26, 2025, 09:00 - 10:00

High temperature superconductors (HTS) in the form of coated conductors are an enabling technology for the next generation of compact nuclear fusion reactors that require higher magnetic fields than Nb3Sn can provide. However, in operation, the superconducting magnet windings will be exposed to a flux of fast neutrons which will introduce structural damage at cryogenic temperatures. Many previous studies using both fission spectrum neutrons and ions at room temperature (or slightly elevated temperatures) have shown that an initial increase in the superconducting current carrying performance upon irradiation is followed at higher fluences by a severe degradation of the properties and eventually complete loss of superconductivity. The superconducting transition temperature is found to decrease monotonically with fluence, strongly suggesting that radiation-induced defects occur throughout the entire crystal lattice, even at relatively low fluence. This talk will outline the research being carried out to improve understanding of radiation damage in HTS materials. This includes innovative in situ ion irradiation experiments to assess radiation damage of HTS at cryogenic temperatures, superconducting property measurements at ultra-high magnetic fields, and studies aimed at elucidating the nature of irradiation induced lattice defects using state-of-the-art microscopy and spectroscopy techniques.

Skyrmions in chiral magnetic multilayers

K Zeissler¹, S. Finizio², L. Huang¹, C. E. A. Barker¹, C. Barton³, K. Fallon⁴, K. Shahbazi¹, E. Haltz¹, T.P. Almeida⁴, J.R. Massey¹, S. Villa⁴, C. Kirkbride⁴, F. Al Ma'mari¹, A.J. Huxtable¹, D. Bracher², A. Kleibert², S. Wintz^{2,5}, S. Mayr^{2,6}, T. Weßels⁷, F. Maccherozzi⁸, B. Sarpi⁸, S.S. Dhesi⁸, A. Sadovnikov⁹, M. Rosamond¹⁰, E.H. Linfield¹⁰, D. McGrouther⁴, S. McVitie¹⁰, T.A. Moore¹, O. Kazakova³, J. Raabe², G. Burnell¹, <u>Christopher Marrows</u>¹

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Plenary Speaker: Christopher Marrows, University of Leeds, UK, June 24, 2025, 16:30 - 17:30

Magnetic skyrmions are topologically-nontrivial spin textures with particle-like properties [1]. Their size, topological stability, and mobility suggest their use in future generations of spintronic devices [2], the prototype of which is the skyrmion racetrack [3]. To realise a racetrack requires three basic operations: the nucleation (writing), propagation (manipulation), and detection (reading) of a skyrmion, all by electrical means.

Here we show that all three are experimental feasible at room temperature in Pt/Co/Ir or Pt/CoB/Ir multilayers in which the different heavy metals above and below the magnetic layer break inversion symmetry and induce chirality by means of the Dzyaloshinskii-Moriya interaction, defining the structure of Néel skyrmion spin textures [4]. We show deterministic nucleation on nanosecond timescales using an electrical point contact on top of the multilayer [5] (Figure 1), current-driven propagation along a wire in which the skyrmions are channelled by defects in the multilayer [6], and their detection by means of the Hall effect (Figure 2) that reveals an unexpectedly large contribution to the Hall signal that correlates with the topological winding number [7].

New directions in skyrmion research include spin wave-driven motion [8] and synthetic antiferromagnetic skyrmions [9].

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- [9] C. E. A. Barker et al., Phys. Rev. B 109, 134437 (2024).

Probing and controlling collective states of 2D quantum materials

Philip King¹

¹University of St Andrews, United Kingdom

Plenary Speaker: Philip King, University of St Andrews, UK (sponsored by M4QN), June 25, 2025, 09:00 - 10:00

Control over materials thickness down to the single-atom scale has emerged as a powerful tuning parameter for manipulating not only the single-particle band structures of solids, but increasingly also their interacting electronic states and phases. A particularly attractive materials system in which to explore this is the transition-metal dichalcogenides (TMDs), both because of their naturally-layered van der Waals structures and the wide variety of materials properties which they are known to host [1,2]. Yet, how the intricate correlated electron states that underpin many of these materials' properties evolve when the compound is thinned to the single-layer limit remains – in many cases – a controversial question. Here, I will discuss our work attempting to address this by integrating monolayer materials growth by molecular-beam epitaxy with electronic structure studies via in situ angle-resolved photoemission (ARPES) and ARPES-based microscopy. I will introduce a new method for achieving enhanced nucleation in monolayer TMD growth, which leads to a step-change in the quality and uniformity of our fabricated samples [3]. I will discuss the resulting electronic structures that we can observe in such epitaxial monolayers, considering, in particular, the controversial charge-density wave phase of monolayer TiSe2 [4-6], exploring the possibility for developing magnetic order in monolayer Cr- and V-based systems [7,8], and uncovering a key role of interfacial coupling in van der Waals heterostructures of 2D quantum materials [9, 10].

This work was performed in close collaboration with A. Rajan, S. Buchberger, S. Mo, N. Kushwaha, O. Armitage, M.D. Watson, T. Antonelli, J. Feng, B. Edwards, Y. in 't Veld, T. Wehling, K. Kovalenka, M.S. Bahramy, P. Wahl, and colleagues from the Universities of St Andrews, Hamburg, Warwick, Manchester, Oxford, Diamond Light Source, Central Laser Facility, and Max-IV synchrotron.

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Studying low-dimensional materials, from fundamental research to real world impact

Prof Chris Howard¹

¹UCL, United Kingdom

Plenary Speaker: Chris Howard, University College London, UK, June 26, 2025, 16:30 - 17:30

Breakthrough theoretical and experimental science around the beginning of the 20th century enabled a bottom-up understanding of condensed matter systems. This foundation enabled the rapid development of new materials and associated technologies, from modern medicine to computing, enormously improving our lives. In this talk, I will explain how my work in studying low dimensional materials [1-3] and contemplating timelines for real-world impact, motivated me to co-found a net-zero technologies 'venture builder' [4] and refocus my fundamental research [5,6].

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[2] Tuning the interlayer spacing of graphene laminate films for efficient pore utilization towards compact capacitive energy storage, Nat Ener. 5, 160 (2020)

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[6] Intermediate-range solvent templating and counterion behaviour at charged carbon nanotube surfaces, Nat. Nano, (2025)

Pressure-quenching as a practical strategy to design new high-Tc conventional superconductors

Prof. Lilia Boeri1

¹Sapienza Università di Roma, Italy

Plenary Speaker: Lilia Boeri, Sapienza Università di Roma, Italy, June 24, 2025, 09:00 - 10:00

Since its discovery over a century ago, superconductivity has promised transformative technologies—lossless power grids, magnetic levitation, ultrasensitive sensors, but the progress in material discovery has been maddeningly slow. Despite decades of attempts, the dream of practical, ambient-condition superconductors has remained out of reach. Eremets' discovery of near room-temperature superconductivity in high-pressure hydrides marked a major turning point in the history of superconductivity, demonstrating that extreme pressure can stabilize phases with unprecedented properties, unthinkable at ambient conditions.[1,2]Ten years after the H_3S discovery, pressure quenching is emerging as a practical strategy to retain high-Tc phases at ambient pressure by preserving structures formed under extreme conditions. In this talk, I will illustrate the conceptual foundation of pressure quenching and present selected applications to systems such as superhydrides,[3] borocarbides,[4] and boron-rich superatomic phases.[5] I will also discuss its broader potential as a synthetic route to ambient-stable superconductors with practical applications.

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Quantum magnetism in the strong spin orbit regime: experimental challenges and opportunities

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Plenary Speaker: Radu Coldea, University of Oxford, UK, June 27, 2025, 09:00 - 10:00

Recent breakthroughs in the theoretical understanding of quantum magnetic materials with strong spin-orbit coupling, where the spin and orbital moment of the electrons are strongly entangled, predict new types of interactions that simply do not exist for "conventional" magnets and thus open up avenues to potentially realize novel forms of cooperative magnetic behaviour ranging from quantum spin liquids to unconventional forms of magnetic orders and dynamics. This talk will review recent progress in the experimental exploration of quantum magnets in this regime using neutron and resonant magnetic x-ray scattering techniques.

Circuits as a simple platform for the emergence of hydrodynamics in many-body systems

Juan Garrahan¹

¹University of Nottingham, United Kingdom

Plenary Speaker: Juan P Garrahan, University of Nottingham, UK, June 25, 2025, 16:30 - 17:30

The emergence of hydrodynamics is one of the deepest phenomena in many-body systems. While the hydrodynamic equations are arguably the most important tools for predicting largescale behaviour, understanding how they emerge from microscopic deterministic dynamics is a century-old problem (despite recent progress in fine-tuned integrable systems). Due to the universality of hydrodynamics, the specific microscopic implementation should not matter. I will describe how classical deterministic circuits provide a minimal, exact, and efficient platform that admits non-trivial hydrodynamics for chaotic systems, and which despite their simplicity manifest a broad range of hydrodynamic behaviours, such as relaxation to Gibbs states, exact Euler equations, shocks, diffusion, and exact KPZ super-diffusion.

Bio: Juan P. Garrahan is a Professor of Physics at the University of Nottingham. His research covers a broad area of theoretical statistical physics and its applications, with particular interests in constrained systems, slow dynamics, the glass transition, quantum non-equilibrium systems, the theory of large deviations, and the statistical mechanics of machine learning. He obtained his PhD from the University of Buenos Aires, was a Glasstone Fellow at the University of Oxford, an EPSRC Advanced Fellow, a visiting professor at UC Berkeley, and a Visiting Fellow at All Souls College, Oxford. At Nottingham he led the Centre for Quantum Non-Equilibrium Systems and currently directs the Machine Learning in Science Initiative.

Invited Speakers

Fingerprints of composite fermion Lambda levels in scanning tunneling microscopy

<u>Professor Zlatko Papic¹</u>, Songyang Pu¹, Ajit C. Balram², Yuwen Hu³, Yen-Chen Tsui³, Minhao He³, Nicolas Regnault^{3,4}, Michael P. Zaletel⁵, Ali Yazdani³

¹University of Leeds, United Kingdom, ²Institute of Mathematical Sciences, CIT Campus, India, ³Department of Physics, Princeton University, USA, ⁴Laboratoire de Physique de l'Ecole normale supérieure, ENS, Université PSL, CNRS, Sorbonne Université, France, ⁵Department of Physics, University of California, USA

Strongly Correlated Electron Systems, June 26, 2025, 14:15 - 16:05

A composite fermion (CF) is a topological quasiparticle that emerges from a nonperturbative attachment of vortices to electrons in strongly correlated two-dimensional materials. Similar to noninteracting fermions that form Landau levels in a magnetic field, CFs can fill analogous "Lambda" levels, giving rise to the fractional quantum Hall (FQH) effect of electrons. Here, we show that Lambda levels can be directly visualized through the characteristic peak structure in the signal obtained via spectroscopy with scanning tunneling microscopy (STM) on a FQH state. Complementary to transport, which probes the low-energy properties of CFs, we show that high-energy features in STM spectra can be interpreted in terms of Lambda levels. We numerically demonstrate that STM spectra can be accurately modeled using Jain's CF theory. Our results show that STM provides a powerful tool for revealing the anatomy of FQH states and identifying physics beyond the noninteracting CF paradigm.

Unconventional π-electron magnetism in graphene nanoribbons

Michele Pizzochero¹

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2D and 1D Materials, June 26, 2025, 14:15 - 16:05

Graphene nanoribbons (GNRs) are a fascinating class of quasi-one-dimensional semiconductors consisting of nanometer-wide strips of hexagonally bonded carbon atoms [1]. Recent advancements in fabrication techniques enabled the realization of atomically precise GNRs with diverse edge geometries, widths, and complex nanoarchitectures [2]. In this talk, I will present graphene nanoribbons as a promising platform for controlling and manipulating unconventional magnetic phases, drawing from both ab initio and model Hamiltonian calculations. First, I will discuss the development of ultra-flat bands and π -electron magnetism in chevron-edged graphene nanoribbons under an external electric field [3]. Second, I will demonstrate the formation of half-semi metallic phases in zigzag-edged nanoribbons upon incorporation into a lateral heterostructure [4, 5]. These findings may open new possibilities for engineering quantum phases in one-dimensional crystals, with potential applications in spintronics and related device concepts.

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Minimal Models for Altermagnetism: Mechanisms and experimental consequences

Andreas Kreisel1

¹University of Copenhagen, Denmark

Magnetism, June 24, 2025, 10:30 - 12:50

The discovery of a new, third fundamental class of collinear magnets with zero net magnetization, but with unconventional spin-polarized band structure, expanded the known classes of ferromagnets and antiferromagnets. The third class, called altermagnet is characterized by spin configurations that remain invariant under a combination of two symmetry operations: time reversal, which flips the spins, and a lattice rotation. This leads to physical properties that are commonly known from ferromagnets, but with a vanishing total magnetization opening the avenue for research directions as for example spintronics, strong correlations and superconductivity, to topological phases of matter [1].

Motivated by the fact that altermagnets generally have paramagnetic states with multiple magnetic ions in the unit cell, we develop a class of minimal models for altermagnetism. These models are applicable to monoclinic, orthorhombic, tetragonal, rhombohedral, hexagonal, and cubic materials and describe d-wave, g-wave, and i-wave altermagnetism.

Having such a minimal model at hand, we examine the origin of the altermagnetic instability, calculate the anomalous Hall effect [2] and emergence of a ferromagnetic order parameter [3]. Concentrating on two-dimensional models in several layer groups that exhibit altermagnetism, we calculate the local density of states in the vicinity of pointlike nonmagnetic impurities and find that the momentum structure of the nodes is directly imprinted on the total local density of states. This signature should be accessible within local probes as scanning tunneling microscopy even without measuring the spin polarization [4].

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[4] Jannik Gondolf, Andreas Kreisel, Mercè Roig, Yue Yu, Daniel F. Agterberg, Brian M. Andersen

arXiv:2502.15606

Probe valency and magnetism of magnetic topological materials using XMCD

<u>Dr Jieyi Liu</u>¹, Tien-Lin Lee¹, Thorsten Hesjedal², Yulin Chen², Gerrit van der Laan¹ ¹Diamond Light Source, United Kingdom, ²University of Oxford, United Kingdom

2D and Topological Physics, June 27, 2025, 10:30 - 12:00

The physical properties of magnetic topological materials are strongly influenced by their nontrivial band topology coupled with the magnetic structure. The focus of this talk is on Co3Sn2S2, a ferromagnetic kagome Weyl semimetal displaying giant intrinsic anomalous Hall effect which can be further tuned via elemental doping, such as Ni substitution for Co. Here, I report a study of Ni-doped Co3Sn2S2 single crystals using synchrotron-based X-ray magnetic circular dichroism (XMCD), X-ray photoelectron emission microscopy (XPEEM), and hard/soft X-ray photoemission spectroscopy (XPS) techniques. I confirm the presence of spin-dominated magnetism from Co in the host material, and the establishment of ferromagnetic order from the Ni dopant. The oxygen-free photoemission spectrum of the Co 2p core levels indicate a Co0+ valency. Surprisingly, I find the electron filling in the Co 3d state can reach 8.7–9.0 electrons in these single crystals. In the remaining part of the talk, I will present the electrical and magnetic characterisation of (Bi1–xSbx)2Te3-intercalated MnBi2Te4 topological insulator multilayers grown by molecular beam epitaxy, particularly by using XMCD to precisely measure the magnetisation of the films. These findings pave the way for the exploration of versatile magnetic topological phases in quantum materials systems.

Understanding the ultrafast electron dynamics and CDW transition in LaTe3 using machine learning

<u>Gesa-Roxanne Siemann</u>¹, Davide Curcio¹, Paulina Majchrzak¹, Charlotte Sanders², Jenny Rigden², Yu Zhang², Deepnarayan Biswas³, Lelie Schoop⁴, Emma Springate², Philip Hofmann¹ ¹Aarhus University, Denmark, ²Central Laser Facility, UK, ³Diamond Light Source, UK, ⁴Princeton University, USA

Computational Physics, June 25, 2025, 10:30 - 12:50

The rare-earth tritelluride LaTe₃ exhibits a unidirectional charge density wave (CDW) with a high transition temperature of 670 K. Recent studies suggest that a short light pulse can not only suppress this primary CDW but also induce a secondary CDW along the perpendicular direction [1]. However, it remains an open question how these structural dynamics affect the electronic structure, and whether signatures of the second CDW can be detected using time- and angle-resolved photoemission spectroscopy. Here, we explore this question, studying the frequency-dependent coherent response of the system, and the time-dependent evolution of the Fermi surface topology, which we compare to predictions by a simple tight-binding model. We support our analysis using *k*-means clustering, a machine learning technique, in order to identify different dynamics throughout the Brillouin zone. This reveals varying relaxation times across the Fermi surface, as well as multiple frequencies that can be ascribed to coherent excitations. [1] A. Kogar *et al.*, *Nat. Phys.* 16, 159–163 (2020).

Can we build a topological qubit in 2025?

Dr Henry Legg¹

¹University of St Andrews, United Kingdom

Nanoscale and 2D, June 24, 2025, 10:30 - 12:50

Recently a lot of attention has been given to the prospects of a realization of a topological qubit based on Majorana Zero Modes. In relation to this, I will critically examine the so-called topological gap protocol (TGP). I will demonstrate that the TGP is not a reliable diagnostic tool for the presence of topological superconductivity and associated Majorana Zero Modes. Moreover, I will show that this protocol is also an unreliable method to detect a superconducting gap, a prerequisite for readout of a well-defined parity in a superconductor and the proposed basis of a putative topological qubit. Based on these insights, I will show that any kind of topological qubit is not possible in the near term.

References:

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[2] Legg, arXiv:2502.19560

[3] Legg, arXiv:2503.08944

Quantifying hydrogen bonding using electrically tunable nanoconfined water

<u>Ziwei Wang^{1,2}</u>, Anupam Bhattacharya¹, Mehmet Yagmurcukardes³, Vasyl Kravets¹, Pablo Díaz-Núñez^{1,2}, Ciaran Mullan¹, Ivan Timokhin^{1,2}, Takashi Taniguchi⁴, Kenji Watanabe⁴, Alexander N. Grigorenko¹, Francois Peeters⁵, Kostya S. Novoselov^{1,2,6}, Qian Yang^{1,2}, Artem Mishchenko^{1,2}

¹The University of Manchester, United Kingdom, ²National Graphene Institute, United Kingdom, ³Izmir Institute of Technology, Turkey, ⁴National Institute for Materials Science, Japan, ⁵University of Antwerp, Belgium, ⁶National University of Singapore, Singapore

Materials for Energy and Chemical physics and Self-Assembly, June 27, 2025, 10:30 - 12:00

Hydrogen bonds (HBs) are critical to both biology and technology, but remain challenging to fully characterize. Existing theories often view hydrogen bonds as electrostatic interactions between positively charged hydrogen atoms and negatively charged acceptors. These models can struggle to accurately capture bond strength, orientation, and cooperative effects, making it difficult to predict the water confinement in complex, hydrogen-bonded systems. In this study, we propose a new model for HBs that treats them as electric dipoles within an external electric field, and produce effective prediction of the bonding environments of water in an electrostatic confining system. The parameters in our model, which relate O-H vibration to HB strength, are calibrated using gypsum—a layered hydrogen-bonded material containing two-dimensional crystalline water-through an externally applied electric field. With the calibrated model, we successfully reproduce many essential properties of confined water reported in the literature. Our approach provides a convenient means of predicting HB-related properties such as bond strength, local electric field, O-H bond length, and dipole moment, by examining the stretching vibration frequency of confined water using non-constructive vibrational spectroscopy. Furthermore, we introduce the concept of hydrogen bond heterostructure, an electrically and chemically tunable material which offers stronger and more directional bonding than conventional van der Waals heterostructures, and holds promise for numerous applications, including catalysis, separation, and energy storage.

Magnificent Magnetic Fields

Amalia Patane¹

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Facilities for CMQM, June 26, 2025, 10:30 - 12:50

Magnetic fields are powerful tools available to scientists for science and technology. They have been crucial for the ground-breaking research that led to several Nobel prizes in Physics, Chemistry and Medicine, most recently for the development of magnetic resonance imaging, MRI (P. Mansfield, University of Nottingham, 2003 Nobel Prize for Medicine) and for research on graphene, the thinnest material (A. Geim and K. Novoselov, University of Manchester, 2010 Nobel Prize in Physics), and will continue to underpin future advances by providing a powerful means of understanding and manipulating matter. The importance of high magnetic fields has been recognized worldwide, including by the USA National Research Council, the European Commission and the EPSRC, which funds the UK Membership of the European Magnetic Field Laboratory (EMFL) since 2015. Amongst the high-magnetic field facilities, the EMFL is a major player on the global scale.

This talk will review opportunities at the EMFL for scientists and technologists across different disciplines (physics, chemistry, biology, and engineering). The user access model of the EMFL provides scientists with free access to state-of-the-art facilities, as well as expert support from the local staff. High-field experiments can be executed with high spatial and energy resolution over a wide range of temperatures down to the millikelvin range, in complex environments, such as high-pressure, and in combination with other large instruments, such as free electron lasers. This research is essential to meet several societal and economic challenges that rely on fundamental science for transformative solutions. As the cost and complexity of high magnetic field installations continues to increase, there is a growing awareness that global collaboration is necessary to maintain the rate of development of new magnets and the dedicated scientific infrastructure around them. The development of such global collaboration is promoted by exchange of data, joint development and production of materials and devices specific for high-field magnets.

Size-restricted magneto-transport in PdCoO₂

<u>Graham Baker</u>¹, Michal Moravec¹, Maja D. Bachmann¹, Aaron L. Sharpe², Nabhanila Nandi¹, Arthur W. Barnard³, Carsten Putzke⁴, Seunghyun Khim¹, Markus König¹, David Goldhaber-Gordon², Philip J.W. Moll⁴, Andrew P. Mackenzie¹ ¹Max Planck Institute for Chemical Physics of Solids, Germany, ²Stanford University, USA, ³University of

Washington, USA, ⁴Max Planck Institute for the Structure and Dynamics of Matter, Germany

Nanoscale and 2D, June 24, 2025, 10:30 - 12:50

The quasi-two-dimensional, delafossite metal $PdCoO_2$ has recently emerged as a benchmark for studying size-restricted transport in complex, high-density metals. This stems from its remarkable low-temperature mean free path of 20 µm and its well-measured, single-sheet Fermi surface. Studies in $PdCoO_2$ thus far have revealed novel and unanticipated features, including transport with reduced symmetry relative to that in the bulk [1,2], as well as the subtlety in distinguishing ballistic and hydrodynamic effects—or even applying this dichotomy at all [3].

Here, we present comprehensive measurements of magneto-transport in PdCoO₂ channels of varying width and orientation, adding cyclotron radius as an additional, experimentally-unable length scale. With increasing magnetic field, we observe first positive and then negative magnetoresistance, both of which depend strongly on channel orientation and become more pronounced with decreasing channel width. Semi-classical simulations establish that magnetoresistance arises from field-induced modification of boundary scattering, and help connect specific features in the data with specific electronic trajectories. Our analysis reveals how, by tuning both channel width and cyclotron radius relative to the mean free path, we are able to obtain information on Fermi surface and scattering anisotropy that is inaccessible to other measurements. We anticipate that this will find application in understanding the microscopic origin of anomalous transport properties in other complex metals.

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Theory of superconducting pairing and topological surface states in UTe2

Professor Brian Møller Andersen¹

¹Copenhagen University, Denmark

Unconventional Superconductivity, June 26, 2025, 10:30 - 12:50

Abstract: "The heavy-fermion compound UTe2 is a candidate for hosting intrinsic spin-triplet superconductivity. At present, however, the type of triplet Cooper pairing realized in UTe2 remains unknown, which calls for further experimental and theoretical investigations. In this talk, I present a

microscopic minimal model for the superconducting phases of UTe2 based on recent findings in the description of its low-energy normal state electronic properties. I apply the resulting theoretical model to extract the nodal gap properties of the allowed superconducting ground states, and deter-mine their associated topological surface states on the experimentally relevant (0-11) cleave plane.

It is found that the Fermi surface of UTe2 enforces additional point nodes in excess to the point nodes imposed by symmetry, which may reconcile several experiments seemingly in conflict with B2u or B3u pairing symmetries. Furthermore, we map out the in-gap Majorana surface-bound modes exist-ing on the (0-11) surface, and discuss their potential for additional insight into the pairing structure of UTe2. Quasiparticle interference (QPI) obtained from scanning tunneling microscopy (STM) is a pow-erful method to help extract the pairing symmetry of unconventional superconductors. We apply the model for UTe2 to compute its QPI signals and compare the resulting QPI with recent STM measurements. We conclude that the two candidate Cooper pair instabilities B2u and B3u exhibit distinct features in the QPI intensity to discriminate these using the experimental data. Characteristic features of the emergent topological

surface states protected by mirror symmetries provide further unique signatures to help pinpointing the pairing symmetry channel of UTe2."

Democratizing nickelates superconductors: Topotactic reduction induced by aluminum sputter deposition

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Unconventional Superconductivity, June 26, 2025, 10:30 - 12:50

After decades of research, a cuprate analog displaying superconductivity was finally found within the nickelate family. It was in 2019 when superconductivity was discovered in infinitelayer (ABO2) nickelates with a critical temperature (TC) around 10-15 K [1]. This discovery has sparked a new realm of research, whose progress is slowed by challenges in materials synthesis and the limited number of research groups capable of producing high quality superconducting samples. The main difficulty lies in the topotactic reduction process required to selectively remove all the apical oxygens from the initial precursor perovskite phase to achieve the superconducting infinite-layer phase, which is typically achieved by an ex situ complex chemical process using CaH2 as the reducing agent. Two alternative in situ reduction methods —metal overlayer deposition via molecular beam epitaxy and atomic hydrogen bombardment— have recently improved this aspect, but their limited accessibility underscores the need for simpler and more reliable methods to facilitate the synthesis of superconducting infinite-layer nickelates.

In this work, we demonstrate the possibility to synthesize high quality superconducting infinitelayer Pr0.8Sr0.2Ni02 thin films by aluminum deposition, using a more accessible technique such as direct current magnetron sputtering [2]. The sputtered aluminum on the parent perovskite thin films pumps the apical oxygen atoms through a redox reaction, transforming the films into the superconducting infinite-layer phase. We systematically optimized the aluminum deposition parameters and compared the superconducting properties of samples reduced through in situ Al deposition with those exposed to air prior to Al reduction (ex situ). In situ Al reduction enhances the quality of the SC Pr0.8Sr0.2Ni02 thin films, with a maximum superconducting transition temperature Tconset of 17 K. This simplified synthesis route, much more accessible than existing methods, offers better control and reproducibility over the topotactic transformation, providing new opportunities to gain insights into the physics of superconductivity in nickelates.

[1] D. Li et al., Nature 572, 62 (2019).

[2] D. Zhang et al., arXiv:2411.04896

Exploring Disorder using Density Functional Theory and X-ray Photoelectron Spectroscopy

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Computational Physics, June 25, 2025, 10:30 - 12:50

While theoretical simulations are routinely performed for interpreting valence X-ray photoelectron spectroscopy (XPS), the interpretation of core XPS primarily relies on comparison to reference spectra. This is challenging, if not impossible, in the case of large molecules or complex solids containing many different local chemical environments, even more so for systems exhibiting disorder. Recently, however, theoretical approaches for calculating core binding energies (BEs) are becoming increasingly common. One approach, based on density functional theory, which has shown great promise for core BE calculations, is DeltaSCF. However, its use in Gaussian basis codes is complicated by the need to use either very large or specifically constructed basis sets which are adapted for core-excited calculations. At the same time, such codes may also suffer from problems such as core-hole hopping, which can lead to poor convergence or inaccurate results. In this talk I will describe an alternative approach, which uses an adaptive multi-wavelet basis to overcome these problems [1]. When combined with a plane-wave basis set approach using core-hole pseudopotentials, it becomes possible to calculate core BEs of both molecules and solids using systematic basis sets, enabling core BE calculations of systems ranging from simple amino acids [1] to disordered molecular [2] and solid state materials [3], offering new opportunities for interpreting core XPS of complex and disordered materials.

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Harnessing Complex Interfacial Flow Dynamics for Structuring Soft Materials

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Non-equilibrium, June 26, 2025, 10:30 - 12:50

Complex multiphase and interfacial flows are important for many processes in nature and industrial applications. Recently we have developed lattice Boltzmann method for simulating complex flow dynamics involving an arbitrary number of fluid components as well as their coupling with solid particle dynamics. In this talk, using lattice Boltzmann simulations, I will discuss two cases where interfacial flow dynamics can be harnessed to structure soft materials. First, to understand the role of the so-called four-colour theorem, we study phase separation dynamics of up to 8 immiscible fluid components. Indeed, we discover that, in 2D, we can suppress droplet coalescence during coarsening when there are 4 or more components and the dynamics become dominated by diffusion. In such cases, the domain size L scales with time t and number of components N as L^3 ~ t/N. Second, we investigate evaporation-driven packing dynamics for colloidal self-assembly. Current experiments typically focus on quasistatic, slow evaporation conditions and ignore particle friction. In contrast, here we demonstrate that by tuning the evaporation rate and interparticle friction coefficient, a range of colloidal cluster configurations-including open, closed, and minimal energy packings-can be accessed. We calculate a dynamic regime diagram. Moreover, force analysis reveals that the packing process consists of two sequential stages: an initial packing stage governed by capillary and hydrodynamic forces, followed by a rearrangement phase dominated by friction. Although frictional forces are relatively small in magnitude, they exert a disproportionately large influence on the final packing outcome. Taken together, tuning the dynamical parameters offers a possible strategy for programmable self-assembly of colloidal clusters.

Harnessing Chirality: Skyrmions as a New Frontier for Quantum Computing

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M4QN II, June 25, 2025, 14:15 - 16:05

Chirality is a fundamental concept in physics, from particle properties to quasi-particles like skyrmions—topologically protected spin textures with twisted configurations defined by helicity. While skyrmion helicity is typically fixed in chiral systems, frustrated magnets offer a new class where helicity becomes a free parameter, leading to richer excitation spectra and complex magnetization dynamics. In the first part of this talk, I will present magnetic nano-skyrmions as candidates for quantum logic elements, emphasizing their potential in quantum computing. Next, I will discuss collective spin-wave excitations around skyrmions in frustrated magnets, highlighting the emergence of dynamical magnon superlattices—localized patterns from interference between extended spin-wave states. These arise from hybridization between the skyrmion's internal modes and extended magnons with a Mexican-hat dispersion. In skyrmion lattices, these localized modes form complex magnonic bands with topological Chern numbers, enriched by long-range interactions. Our findings reveal a rich interplay between frustration, topology, and dynamics, paving the way for skyrmion-based magnonic devices beyond the chiral paradigm.

Altermagnetism imaged and controlled down to the nanoscale

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Magnetism, June 24, 2025, 10:30 - 12:50

Altermagnetism is a newly identified class of magnets which combines properties from both ferromagnets and antiferromagnets, making them highly promising candidates for spintronic applications[1,2]. We recently demonstrated the spin split nature of the altermagnetic electronic band structure in MnTe[3]. In this work, we demonstrate that the unique resultant properties of altermagnets can be used to image them in unprecedented details, and also to control them in unique ways.

Utilising a combination of linearly and circularly polarised x-rays, in a single instrument, we generate a full Neel vector map of the magnetic domain in MnTe, showing all 6 domain types and revealing vortices and their vorticity. In addition, we utilise a combination of patterning and field cooling to nucleate single domains of our choosing from the micron to nanoscale. We also show generation and control of the position and vorticity of single vortices. These experiments showcase the unique properties of altermagnets and also provide a platform for the next stages of research and application[4].

Extracting spin from compensated magnets at picosecond timescales

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M4QN I, June 25, 2025, 10:30 - 12:50

Interfaces in heavy metal – antiferromagnet heterostructures have recently become highly investigated and debated systems in the effort to create spintronic devices that function at terahertz frequencies. Such heterostructures have great technological potential because antiferromagnets can generate sub-picosecond spin currents which the heavy metal can convert into charge signals. In this talk I will present our recent work on the optically induced picosecond spin transfer from magnetically compensated magnets, including antiferromagnets and ferromagnetic alloys, to Pt using time-domain THz emission spectroscopy. We will focus on three studies in antiferromagnetic insulators KCoF3 and KNiF3, in antiferromagnetic metal FeRh, and rare earth-transition metal alloy CoGd. Through our studies, we are able to shed light on the microscopy of spin transfer at picosecond timescales and identify key figures of merit for its efficiency.

Topological excitons in 1D

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M4QN I, June 25, 2025, 10:30 - 12:50

Topological band theory has celebrated various successes over the last few years, such as the recent classifications of crystalline materials based on their space group symmetry. We are currently witnessing a drive to generalise this theory to the case where interactions between electrons become relevant, with much work focused on ground states. As an alternative direction, we here study the topology of interaction-induced excitations, specifically excitons in semiconductors. In my talk, I will give a pedagogical introduction to the classification and bulk-boundary correspondence of exciton band structures based on inversion symmetry.

Room temperature spin nematic phase and anomalous Hall effect in tetragonal lattice AMnBi2 (A = Ca, Yb)

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China, ⁸RIKEN, Japan, ⁹Smalley-Curl Institute, Rice University, United States

2D Materials, June 25, 2025, 14:15 - 16:05

A nematic phase is a state where elongated molecules in liquid crystals exhibit no crystalline positional order but are aligned with their long axis approximately parallel to form directional order with twofold (C_2) rotational symmetry. A spin nematic phase is a magnetic analogue of classical liquid crystals, where spins are spontaneously entangled to form anisotropy in spin space without breaking the time reversal (T) symmetry. On the other hand, the order parameter characterizing the T-symmetry breaking is the scalar spin chirality (SSC) χ ijk=(S i(S j×S k)). where S_i, S_j, S_k are spins at neighboring sites i, j, k, respectively4-6, and nonzero SSC is known to induce anomalous Hall effect (AHE). Although a spin nematic phase has been suggested in the frustrated magnets and the square-lattice iridate, how a spin nematic phase might affect magneto-transport properties is unknown. Here we use polarized neutron scattering to show that tetragonal lattice AMnBi2 (A=Ca,Yb) is strictly a c-axis aligned collinear antiferromagnet (C-type) with T N≈270 K and 290 K. On cooling from 450 K to T N, low-energy spin excitations in YbMnBi2 spontaneously change from isotropic to anisotropic in spin space, forming a dynamic spin nematic phase around 400 K, before gapping out below T N. Under an in-plane external magnetic field, the Yb3+ moments interact with the dynamic spin nematic phase to induce nonzero SSC, giving rise to AHE8 and anomalous Nernst effect (ANE) in YbMnBi2 that is absent in CaMnBi2 above T_N. Our results, therefore, provide compelling evidence for dynamic SSC-induced AHE and ANE in the paramagnetic phase of a compensated collinear antiferromagnet, and offer a new avenue towards room temperature fast spintronics without magnetic order.

Spinon Mediation of Witness-Spin Dynamics and Ground State in Herbertsmithite

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Frustrated Magnetism and Spin Ice, June 27, 2025, 10:30 - 12:00

The kagome lattice of spin-1/2 Cu atoms in herbertsmithite (ZnCu3(OH)6Cl2) is conjectured to sustain a quantum spin liquid (OSL) state with spinon quasiparticles. Each kagome plane is separated from its homologues by a layer of spinless Zn atoms. Providentially, however, some spin-1/2 Cu atoms substitute randomly onto these inter-kagome Zn sites. We reconceptualize these 'impurity' atoms as 'witness-spins' that provide an exceptional new interrogative of the OSL state. To explore herbertsmithite witness-spin dynamics in this context introduce spinnoise spectroscopy1-4 to QSL studies. It reveals the existence, slowing and intensification of spin noise, prefatory to a sharp transition at T^{*}≈260 mK. Below T^{*} the spin-noise power spectral density $S(\omega,T) \propto \omega^{(-\alpha(T))}$ stabilizes at $\alpha \approx 1$; the spin noise variance σ M^2 (T) diminishes precipitously; the ultra-low-field magnetic susceptibility $\chi(T)$ undergoes a sharp transition into a phase exhibiting an Edwards-Anderson order-parameter and ultra-slow spinstate ageing. To understand these phenomena we introduce a model of spinon-mediated witness-spin interactions which, despite having only one free parameter, corresponds demonstrably to all these experimental observations. The model predicts dramatic slowing and intensification of the witness-spin fluctuations and noise spectrum $S(\omega,T)$ with cooling; this presages a transition into a unique spinon-mediated phase signified by rapidly diminishing spin noise, conversion to $S(\omega,T) \propto \omega^{(-1)}$, a sharp cusp in the DC magnetic susceptibility $\chi(T)$, the appearance of an Edwards-Anderson spin-glass order-parameter. Hence, the empirical phenomenology of witness-spin noise represents spinon-mediation of witness-spin dynamics, leading to both a unique quantum entangled witness-spin-glass ground state, and coterminous quantification of the spinon spectrum in herbertsmithite.

Excelling in Photoemission Spectroscopy at Diamond Light Source

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Facilities for CMQM, June 26, 2025, 10:30 - 12:50

Several beamlines at the Diamond Light Source pair photoemission spectroscopy with the intensity and flexibility of synchrotron radiation to enable experiments across materials science, organic and inorganic chemistry, surface science, condensed matter physics, and more. In this talk I will give some brief historical context, review the facilities available and user access routes at Diamond, and then focus on two beamlines with recent developments of interest to the CMQM community. IO9 has recently developed a "momentum microscope" enabling efficient and bulk-sensitive measurements in the soft x-ray regime. At IO5, micro- and nano-ARPES experiments now routinely enable the characterisation of samples and sample environments previously considered unsuitable for ARPES, and also deliver new insights on more traditional single crystal samples. Exemplifying this, I will show new micro-ARPES results on Ta dichalcogenides, where a charge density wave with a previously unreported periodicity is found in certain minority regions of heterogeneous crystals.

Predictive Modeling of Superconductors: From High-Pressure Hydrides to Nickelates

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Superconductivity I (IOP SC Group), June 24, 2025, 10:30 - 12:50

Predictive modelling of superconductors has long been a central goal in condensed matter physics. For conventional phonon-mediated superconductors, theoretical frameworks now reliably describe the superconducting transition temperature (Tc), even in complex materials. However, a major challenge remains in accurately determining the precise crystal structures that correspond to experimental observations—particularly in the field of high-pressure hydride superconductors. Lutetium hydride is a recent notorious example highlighting the difficulty of identifying experimentally synthesised structures under pressure. I will present an alternative approach based on its intriguing pressure-induced colour changes [1], demonstrating how colour can serve as an intuitive descriptor in predictive modelling to guide experiments in structure identification of high-pressure hydrides.

In contrast, predicting Tc for unconventional superconductors is an extremely challenging task, largely because even understanding their normal state properties remains incomplete. This lack of fundamental insight into the normal state hinders efforts to model and predict new unconventional superconductors. Growing evidence suggests that many of these materials share a common phenomenology in their phase diagrams, including pseudogap phases, strange metal behaviour, and other correlated electronic states where spin fluctuations play a crucial role. Understanding these complex phase diagrams is therefore essential for developing predictive models of unconventional superconductivity. Using dynamical mean-field theory, I will present how spin fluctuations give rise to novel spin-phonon coupling in nickelate superconductors—a phenomenon that may be universal in the normal state of unconventional superconductors modeling of this challenging class of materials.

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Fabrication of atomic-scale devices in silicon for quantum computing

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M4QN I, June 25, 2025, 10:30 - 12:50

Atomic-scale devices made from individual dopant atoms in silicon offer a wealth of opportunities to study new physical phenomena and to create novel technologies. For example, either the valence electron spin and nuclear spin of a single dopant can form the qubit in a silicon-based quantum computing architecture, and artificial lattices of individual dopant atoms can provide the basis for analogue quantum simulators. The deterministic placement of single dopant atoms at nearly exact lattice sites is possible using the technique of scanning tunnelling microscopy hydrogen resist lithography. However, until recently there have been limits to the single-atom fabrication yield, a severe hinderance to device scaling. I will explain how we have overcome these limits, and show that using arsenic-in-silicon it is possible to achieve a single-atom yield approaching 100%, providing a fabrication pathway to the scaling of single-atom devices [1,2]. Additionally, I will describe our device fabrication effort and show preliminary electrical measurements from arsenic-in-silicon devices made using hydrogen resist lithography. Finally, I will briefly show how extreme ultraviolet (EUV) lithography can be used to selectively remove the hydrogen resist, offering a route to fabricating interconnects for atomic-scale devices, across an entire wafer [3].

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As simple as one, two three? Probing self and collective dynamics by counting colloids

Alice Thorneywork1

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Statistical and Nonlinear, June 25, 2025, 10:30 - 12:50

For more than a hundred years, scientists have carefully analysed the apparently random fluctuations in Brownian trajectories to learn about soft systems. In a more general sense, however, the information hidden within experimental fluctuations is typically underexploited, due to challenges in unambiguously linking fluctuation signatures to underlying physical mechanisms. In this talk, I will discuss our recent work developing new approaches to interpreting fluctuations in experimental data from a variety of soft systems, and thereby turn 'noise' into signal. In particular, I will share some recent results taking a fresh look at fluctuations in equilibrium colloidal monolayers. Here, we have combined experiment, simulation and theory to explore how simply counting colloids can reveal details of self and collective dynamics. I will then discuss ongoing work to extend this understanding to driven systems [2,3], with the long-term goal of elucidating characteristic fluctuations in our synthetic nanopore experiments [4].

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Electronic response to a current-induced insulator-to-metal transition in Ca2RuO4

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Strongly Correlated Materials, June 24, 2025, 14:15 - 16:05

Layered perovskite ruthenates exhibit a host of different electronic phenomena due to the intertwined charge, lattice, spin and orbital degrees of freedom in these systems. Such a rich phenomenological landscape is evidence of the close competition of energy scales in these materials, which in turn makes them highly susceptible to various external perturbations. A common feature across the materials family is the sensitivity of the electronic ground state to the rotations and distortions of the RuO6 octahedra, with a prime example being the singlelayer Ruddlesden-Popper calcium ruthenate, Ca2RuO4. It enters an orbitally selective Mott insulator state below 357 K, but can be driven through an insulator-to-metal transition by many other tuning parameters, such as chemical substitution, pressure, strain and electric fields. More unconventionally, Mott insulating Ca2RuO4 can also be driven into a metallic phase by DC current. While the zero-current transition is understood to originate from a distortion in the RuO6 octahedra, the effect of the current on the electronic structure and the mechanism by which it induces an insulator-to-metal transition remain unclear. I will show how we used carefully designed photoemission experiments, where current was passed through the sample in situ, to directly probe the electronic structure changes across the current-induced transition [1]. Our results demonstrate that the current-induced phase is electronically distinct from the high-temperature zero-current metallic phase, and highlight the strong interplay of lattice and orbital effects in the electronic response.

[1] Suen, C.T., Marković, I., et al. Nat. Phys. 20, 1757 (2024)

Spin-orbital phases in 4d pyrochlore oxides

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Spin-Orbit, June 24, 2025, 14:15 - 16:05

Complex ruthenium compounds serve as a platform for a plethora of exotic elec-tronic phases arising from the interplay of not only Coulomb repulsion, bandwidth or crystal eld, but also sizeable spin-orbit coupling. The delicate balance between these interactions can be controlled by selecting suitable lattice structures. In ruthenates, the key building block is the octahedrally coordinated Ru4+ ion, hosting a spin-orbit-entangled Jeff = 0 singlet. Although this singlet is non-magnetic, strong inter-site

interactions can induce a quantum phase transition to magnetic order through the condensation of excited states, termed excitonic magnetism. In a layered perovskite structure with corner-sharing octahedra and 180° RuORu bonds, strong magnetic exchange leads to excitonic magnetic order. Weakening this exchange to approach a quantum critical point could give rise to another exotic magnetic state. A promising structural framework for ne-tuning magnetic exchange is the pyrochlore lattice, such as that found in pyrochlore ruthenates A2Ru207 (A = Y, rare earth). A2Ru207 host RuORu bond angles of 130°, resulting in weaker exchange. The geometric frus-tration should further suppress long-range magnetic order. Nonetheless, A2Ru207 compounds exhibit long-range magnetic order at low temperatures, likely representing marginal excitonic magnets near a quantum critical point.

I will discuss our approach to drive a pyrochlore ruthenate to the limit by em-ploying a small "spectator" A cation with covalent bonding with oxygen. With high pressure synthesis, we discovered new pyrochlore ruthenate In2Ru207. However, instead of excitonic magnetism, an emerging valence bond solid instability stabilises and unexpected "orbital molecule" state [1].

[1] A. Krajewska et al., Science Advances 10, eadn3880 (2024).

Condensed Matter and Quantum Materials Research at ISIS Neutron and Muon Source

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Facilities for CMQM, June 26, 2025, 10:30 - 12:50

Neutrons and muons are two important probes used in the investigation of condensed matter and quantum materials. The ISIS Neutron and Muon Source hosts several beamlines dedicated to exploring the structure and properties of these materials. These beamlines, often referred to as "super microscopes," are optimised to study a wide range of matter, including condensed matter, organic materials, quantum materials, thin films, surfaces, and catalysts.

In this talk, we will provide a brief overview of the available facilities and highlight recent research achievements. Our focus will be on beamlines that utilise neutron spectroscopies to investigate the microscopic properties of quantum and energy materials, complemented by data analysis and interpretation through quantum mechanical simulations. Selected case studies will be presented in detail on ferroelectric materials, quantum spin liquids and on battery materials. We will demonstrate that neutron spectroscopies are essential for probing the dynamics of these materials, which cannot be explored by other means.

Programming Self-Assembly for Colloidal Photonic Crystals

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Statistical and Nonlinear, June 25, 2025, 10:30 - 12:50

Colloidal particles in the size range of hundreds of nanometres appeal as building blocks for photonic crystals with a complete photonic band gap in the visible [1]. The self-assembly of colloidal photonic crystals – touted as a low-cost, scalable fabrication technique – has, however, proved elusive [2,3]. Diamond-structured colloidal photonic crystals, which have been much sought-after over the past three decades [4,5], continue to prove challenging targets for being realised at scale via programmed self-assembly. In this presentation, I will demonstrate, using a variety of computer simulation techniques, how hierarchical self-assembly pathways can be programmed, and medium-range order can be encoded in designer patchy particles for facile self-assembly of colloidal photonic crystals [6-10], in close connection with recent experimental breakthroughs [11,12]. I will highlight how certain long-standing challenges have been addressed to push the frontiers of colloidal self-assembly.

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Gauge freedoms in unravelled quantum dynamics: How do different continuous measurements yield identical quantum trajectories and what does it mean for their symmetries?

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Non-equilibrium, June 26, 2025, 10:30 - 12:50

Quantum trajectories of a Markovian open quantum system arise from the back-action of measurements performed in the environment with which the system interacts. In this talk, I will consider counting measurements of quantum jumps – corresponding to different representations of the same quantum master equation – and present necessary and sufficient conditions under which these different measurements give rise to identical ensembles of quantum trajectories. I will then apply these results to characterise how weak unitary symmetries of the quantum master equation governing the average dynamics of the system can be retained by the stochastic dynamics of quantum trajectories and discuss their consequences for numerical simulations.

Towards Skyrmionic Artificial Synapses for Neural Network Hardware

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M4QN II, June 25, 2025, 14:15 - 16:05

The rapid rise of resource-intensive artificial intelligence (AI) has created an urgent need for next-generation computing hardware that combines high performance with improved energy efficiency—key to enabling sustainable AI. This is especially important in domains such as healthcare, automation, and robotics, where low latency and data privacy are essential. The human brain, consuming only ~20 W, remains the benchmark for versatile and efficient information processing.

Magnetic skyrmions—topologically protected spin textures that behave as mobile quasiparticles—are promising candidates as information carriers for brain-inspired hardware. Their robustness and controllability make them attractive for intelligent computing, including implementations in reservoir computing and magnetic synapses.

We previously proposed: (i) an all-magnetic skyrmion-based topological multiplexing device that functions as an interconnect, exploiting topological filtering via the skyrmion Hall effect; and (ii) a skyrmion-based artificial synapse that numerically demonstrates synaptic weight encoding in a thermally stable magnetic multilayer. This synapse consists of a racetrack divided into preand post-synaptic regions by a magnetic barrier. Spin–orbit torques (SOTs) drive skyrmions across this barrier, modulating conductance to emulate long-term potentiation and depression. Here, we present recent experimental progress. We have fabricated a device based on our synapse design using [Pt/CoFeB/Ir]₈ multilayers, characterised it via magnetic force microscopy and magneto-optic Kerr effect imaging, and demonstrated thermally induced skyrmion nucleation at notch-like constrictions and their current-driven motion. Informed by micromagnetic simulations and early experimental results, we outline a behavioural circuit model of our synapse to explore its integration into future neural network hardware for ultra-energy-efficient inference.
Ultraclean van der Waals Heterostructures

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2D Materials and Toplogical Devices, June 24, 2025, 14:15 - 16:05

Layer-by-layer assembly of van der Waals (vdW) heterostructures underpins new discoveries in solid state physics, material science and chemistry. Despite successes, all current assembly techniques use polymeric supports which limit their cleanliness, ultimate electronic performance, and potential for optoelectronic applications. In the first part of the talk, I will introduce a polymer-free platform for heterostructure assembly using re-usable flexible silicon nitride membranes. This approach enables production of heterostructures with interfaces free from interlayer contamination and correspondingly excellent optoelectronic behaviour. In addition, eliminating polymeric supports allows new possibilities for vdW heterostructure fabrication: assembly at temperatures up to 600 °C, and in different environments including ultra-high vacuum and liquid submersion.

In the second part, I will discuss how this new technology affects twisted bilayer TMDs in the regime of small twist angles. Here I will cover the atomic reconstruction: formation of ferroelectric domains in TMDs with different thicknesses and explore how their atomic structure can be characterised using multi-slice electron ptychography. I will also show our recent results on ferroelectric tunnelling junctions and their string dependence on the pre-existing domain network. In the last, conclusive part I will discuss the challenges the field is facing, using devices based on twisted 2D interfaces as an example. I will show the importance of nanofabrication in the context of twistronics and offer avenues for future development of nanofabrication pathways.

Silicon qubits fabricated using industrial 300mm wafer processes

Dr. Ross Leon¹

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M4QN II, June 25, 2025, 14:15 - 16:05

Spin qubits based in silicon offer advantages of low spin-orbit coupling and low concentration of nuclear spins leading to long coherence times and high fidelity operations. In addition, they offer potential compatibility with the high-yield fabrication processes of the semiconductor industry, particularly for architectures based on existing silicon metal-oxide-semiconductor (MOS) technology, supporting scalability as well as integration of quantum and classical electronics. I will present recent progress in fast, high-fidelity readout of MOS spin qubits produced using industrial grade 300 mm wafer processes, achieving using compact qubit sensors that can be readily incorporated within qubit arrays. I will also discuss the integration of quantum dots with digital and analogue CMOS electronics operating below 1K, enabling rapid electrical characterisation of over 1024 addressable quantum dots and prospects for the future development of this technology.

Oral Presentations

Orbital Rashba induced triplet superconductivity in elemental superconductors

Thomas Saunderson^{1,2,3}, Martin Gradhand¹, Dongwook Go^{1,2}, James F. Annett⁴, Maria Teresa Mercaldo⁵, Mario Cuoco^{5,6}, Mathias Kläui^{1,7}, Jacob Gayles^{3,2}, Yuriy Mokrousov^{1,2} ¹Johannes Gutenberg-University Mainz, Germany, ²Peter GrÅNunberg Institut and Institute for Advanced Simulation, Germany, ³University of South Florida, United States, ⁴University of Bristol, United Kingdom, ⁵Universit`a di Salerno, Italy, ⁶SPIN-C, Italy, ⁷Norwegian University of Science and Technology, Norway

Spin-Orbit, June 24, 2025, 14:15 - 16:05

Modern computation must adapt to meet the challenges of the new era. The energy demands of AI technology are juxtaposed with the fears of global warming. This, coupled with Moore's law breaking down, shows that radical change to computer architectures is essential. Recent advancements in orbitronics demonstrate remarkable efficiency gains using costeffective materials [1], while spin-Hall mediated responses notably intensify near the superconducting transition [2]. Breaking inversion or time-reversal symmetry efficiently extracts these unconventional currents, however for material-specific predictions first principles techniques are essential.

In this talk I will discuss recent work [3] where we show from first principles the existence of supercurrent-driven spin triplet densities on the surface of a variety of simple superconducting materials irrespective of the strength of spin-orbit coupling. We are able to attribute this phenomenon to the superconducting non-relativistic orbital Rashba Edelstein effect. Furthermore, we find that the spin-orbit induced spin moment is one order of magnitude smaller than the orbital moment, and has a vanishing effect on the total magnitude of the induced triplet density. Our findings imply the existence of a route to generate spincurrents without the use of heavy metals. Additionally, as an orbital moment can couple directly to a magnetic field, it shows that orbital physics is the dominant term that drives the superconducting diode effect.

[1] YG Choi et al, Nature 619, 52 (2023)

- [2] KR Jeon et al, ACS Nano 14, 15874 (2020)
- [3] TG Saunderson et al, arXiv:2504.01271

Phonon-Limited Conductivity of Topological Surface States in Bi₂Se₃

<u>Miguel Luque Canete</u>¹, Ivana Savic¹ ¹King's College London, United Kingdom

2D and Topological Physics, June 27, 2025, 10:30 - 12:00

Topological insulators, such as Bi_2Se_3 , exhibit topological surface states (TSS) with promising applications where understanding their electronic transport properties is essential. At room temperature, phonon interactions could significantly impact the conductivity of TSS, yet the nature of the phonons and the magnitude of the effects remain unclear. In this work, we develop and validate a framework to compute the phonon-limited conductivity of the Bi_2Se_3 TSS using the Boltzmann transport equation in the relaxation time approximation, including scattering with acoustic, non-polar and surface polar optical phonons. In particular, we introduce a rigorous model to account for surface optical phonon scattering using the dielectric continuum model. All physical parameters entering the framework can be obtained from ab initio calculations. Applying the framework to Bi_2Se_3 TSS, we quantify scattering rates arising from distinct phonon modes and evaluate their contributions to the temperature-dependent transport properties of TSS. Our findings suggest that the dominant scattering mechanism is acoustic phonon scattering.

Coherent phonon dynamics in two-dimensional charge density wave materials

<u>Enrico Da Como¹</u>, Charles Sayers², Ettore Carpene², Giulio Cerullo², Yu Zhang³, Charlotte Sanders³, Emma Springate³

¹Department of Physics, University Of Bath, United Kingdom, ²Politecnico Milano, Italy, ³Central Laser Facility, Research Complex at Harwell, STFC Rutherford Appleton Laboratory, United Kingdom

Non-equilibrium, June 26, 2025, 10:30 - 12:50

We present femtosecond time- and angle-resolved photoemission spectroscopy combined with computational methods to investigate the coherent lattice dynamics of prototypical CDW systems based on 1T-TaSe2. The photo-induced temporal evolution of the periodic lattice distortion associated with the amplitude mode reveals the dynamics of the free energy functional governing the order parameter. Our approach establishes that optically-induced screening rather than CDW melting at the electronic level leads to a transiently modified potential which explains the anharmonic behaviour of the amplitude mode and discloses the structural origin of the symmetry-breaking phase transition (1).

We also present data on the origin of its CDW gap and discuss the interplay between electronphonon coupling and Mott physics in this interesting material (2),

(1) Sayers et al. Communications Physics, 7, 389 (2024)

(2) Sayers t al. Physical Review Letters, 130, 156401 (2023)

Crystallographic orderings in the AlTiVNb and AlTiCrMo refractory highentropy superalloys: first-principles theory and atomistic simulations

<u>Dr Christopher Woodgate</u>¹, Hubert Naguszewski², David Redka^{3,4}, Ján Minár⁴, David Quigley², Julie Staunton²

¹School of Physics, University Of Bristol, United Kingdom, ²Department of Physics, University of Warwick, United Kingdom, ³Department of Applied Sciences and Mechatronics, Munich University of Applied Sciences (HM), Germany, ⁴New Technologies Research Centre, University of West Bohemia, Czech Republic

Computational Physics, June 25, 2025, 10:30 - 12:50

Refractory high-entropy superalloys (RSAs) are metallic alloys containing aluminium and at least three further early transition metal elements. Although in general high-entropy alloys are expected to form single-phase solid solutions in which all lattice sites have uniform probabilities of being occupied by different elements, the addition of AI as an alloying element is understood to promote the formation of crystallographically ordered structures. Here, we combine ab initio electronic structure calculations, a concentration wave analysis, and atomistic simulations to examine the phase stability of two prototypical RSAs: AlTiVNb and AITiCrMo [1]. In alignment with experimental observations, we predict B2 crystallographic orderings emerging at high temperatures in both alloys, as well as eventual decomposition into multiple competing phases with decreasing temperature. We interpret these findings in terms of the alloys' underlying electronic structure, with hybridisation between the sp states of Al and the d states of the transition metals understood to play an important role. We then examine the impact of these crystallographic orderings on the alloys' residual resistivity. Counterintuitively, for both alloys, we find that the emergence of (partial) long-range crystallographic order results in an increase in residual resistivity. We understand this increase as originating in a reduction in the electronic density of states at the Fermi level induced by the ordering, as well as qualitative changes to the nature of the alloys' smeared-out Fermi surfaces.

[1] C. D. Woodgate, H. J. Naguszewski, D. Redka, J. Minar, D. Quigley, J. B. Staunton, arXiv:2503.13235.

Physical properties of layered metal-rich chalcogenides Ta2Se and its application

Jeongmin Lee¹, Kimoon Lee¹ ¹Kunsan National University, South Korea

2D and 1D Materials, June 26, 2025, 14:15 - 16:05

Transition metal-rich chalcogenides (TMRCs) have emerged as promising candidates for novel quantum materials due to their dense transition-metal layered structures, which can induce unique electronic and optical properties. In this study, we investigate the structural, electronic, and vibrational properties of Ta₂Se, a layered TMRCs, and reveal an unconventional energy level configuration arising from its densely packed Ta-layer units. X-ray diffraction and energy-dispersive X-ray spectroscopy confirm the structural and chemical composition of the synthesized Ta2Se single crystal. Electrical transport measurements indicate metallic conduction with a high hole carrier concentration of 2×10^{21} cm⁻³.

Polarized Raman spectroscopy identifies two distinct Raman-active modes at 183 cm⁻¹ and 212 cm⁻¹, both assigned to A₁g vibrational symmetry. Furthermore, ultraviolet photoemission spectroscopy and impedance spectroscopy determine the work function of Ta2Se to be 3.6 eV, which is significantly lower than that of elemental Ta. Using this low work function characteristic, a Ta₂Se/p-Si metal/Schottky junction was fabricated, demonstrating rectifying behavior and prospective use in next-generation electronic appliances. This study offers a new understanding of the phonon vibration, charge transport, work function, and their connections.

A comprehensive study on the multi-band emission of zinc sulfide thin film grown by aerosol-assisted chemical vapour deposition

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Thin-Films, June 25, 2025, 14:15 - 16:05

zinc sulfide (ZnS) is well known due to its wide band gap of ~3.7 eV and high exciton binding energy of 40 meV at room temperature. Its abundant nature and low toxicity compared to its cadmium sulfide counterpart make it one of the most promising materials for industrial applications in ultraviolet light-emitting diodes, electroluminescence devices, photocatalysts, optoelectronics and biodevices. Typically, hexagonal wurtzite phase ZnS forms at temperatures over 1000 °C. In this work, the hexagonal wurtzite phase of crystalline ZnS film has been synthesized using a low-temperature (T = 350 °C) aerosol-assisted chemical vapour deposition (AACVD) method utilising zinc diethyldithiocarbamate [Zn(S2CNEt2)2] as a single source precursor. The as-grown ZnS film has been analyzed by scanning electron microscope (SEM), energy dispersive X-ray (EDX), Raman, and X-ray photoelectron (XPS) spectroscopies, and powder X-ray diffraction (p-XRD) to elucidate film morphology, chemical composition, and crystal structure. EDX and XPS analysis showed that Zn-rich in the ZnS thin film. Photoluminescence spectra of the as-grown ZnS revealed defect-induced high-intensity multiemission in the visible region, below the band gap energy of ZnS. The origin of these exciton recombination mechanisms was confirmed by density functional theory (DFT). These results highlight the potential of AACVD-grown ZnS for efficient multi-band light emitters in a wide wavelength range from UV to visible regions of the electromagnetic spectrum.

Linear-time classical approximate optimization of cubic-lattice classical spin glasses

Adil Gangat

¹Caltech, United States, ²NTT Research, Inc., United States

Frustrated Magnetism and Spin Ice, June 27, 2025, 10:30 - 12:00

Computing low-energy configurations (i.e., approximate optimization) of classical spin glasses is of relevance

to both condensed matter and combinatorial optimization. Recent theoretical work opens the possibility to make its time complexity with quantum annealing generically polynomial, and D-Wave experiments can now achieve approximate optimization of cubic-lattice classical Ising spin glasses with $\sim 10^{4}$ spins. It is therefore

timely to ask which short-range classical spin glasses are good candidates for demonstrating quantum advantage in the time complexity of heuristic approximate optimization. One intuition is to consider models with very rugged energy landscapes in configuration space. However, here we provide evidence that short-range classical spin glasses may be approximately optimized in linear time and space with a very simple deterministic tensor-

network heuristic regardless of ruggedness. On the cubic lattice with up to $50 \times 50 \times 50$ spins, we obtain energy errors of ~3% for the ±J model used in recent D-Wave experiments, and ~5% for much more rugged planted-solution instances. For cubic-lattice-lsing reductions of unweighted Max-Cut on random 3-regular graphs with up to 300 vertices, we find energy errors of <1% and approximation ratios of about 72-88%. These results inform the search for quantum advantage and suggest an efficient classical method for generating warm starts for other spin-glass optimization algorithms. Our algorithm is amenable to massive parallelization and may also allow for low-power, accelerated implementations with photonic matrix-multiplication hardware.

Momentum-dark excitons & trions in systems exhibiting a Mexican-hat energy dispersion: example of InSe

Lewis Burke¹, Mark Greenaway¹, Joseph Betouras¹ ¹Loughborough University, United Kingdom

2D and 1D Materials, June 26, 2025, 14:15 - 16:05

Monolayer Indium Selenide (InSe) is a 2D metal chalcogenide which exhibits an inverted Mexican-hat-shaped energy dispersion in the valence band and a parabolic-shaped conduction band close to the Γ -point [1]. In this system, the electron and holes that couple to create the lowest energy exciton and trions reside at different points in momentum space. This results in the ground state of these quasiparticles being known as momentum-dark due to their much-reduced coupling to light. Thus, they require external processes to enable this coupling. As a result, these states often have a much longer lifetime compared to their bright counterparts.

We investigate the properties of these states by employing variational techniques and explore the "brightening" of such states via the inclusion of phonon coupling [2]. To achieve this, we use the dominant phonon coupling of InSe (longitudinal acoustic [3]), which can transfer the required momentum and energy to transform the states from being momentum-dark to a virtual bright state. This allows us to study the effects such states have on the photoluminescence spectrum of the material as a function of temperature.

References

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[2] L. J. Burke, M. T. Greenaway, and J. J. Betouras, arXiv:2502.06473 (2025)

[3] N. T. Paylaga, et al. npj 2D Materials and Applications, 8(1),12 (2024)

Momentum-space modulated symmetries in the Chiral Luttinger liquid

<u>Alexandre Chaduteau</u>¹, Nyan Raess¹, Henry Davenport¹, Frank Schindler¹ ¹Imperial College, United Kingdom, ²Royal Holloway University of London, United Kingdom

Strongly Correlated Materials, June 24, 2025, 14:15 - 16:05

The chiral Luttinger liquid is a 1-dimensional model of strongly-correlated electrons that develops quantum chaos as soon as a—however slight—nonlinear dispersion is introduced for the microscopic electronic degrees of freedom. In my talk, I will explain how we can identify an infinite family of translation-invariant interaction potentials with corresponding modulated symmetries. These symmetries are highly unconventional: they are modulated in momentum space (and do not seem to have an easy physical interpretation). I will develop a systematic understanding of these symmetries and study the resulting blocks in the Hamiltonian. These blocks are reminiscent of Hilbert space fragmentation in that, even though they are labeled by a symmetry, this symmetry is highly nonlocal and does not have a simple interpretation. (This talk is based on arXiv: 2409.10359.)

High Sensitivity Broadband Fibre-Integrated Waveguide Magnetometry in Diamond

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M4QN I, June 25, 2025, 10:30 - 12:50

Quantum emitters have gained significant attention for their applications in quantum sensing and photonic technologies. They are able to function with high sensitivity at room temperature. In particular, the negatively charged nitrogen-vacancy (NV) colour centre in diamond has been utilised for its optically accessible electron spins. The NV centre has potential as a solid state electron spin-based sensor capable of sensing temperature as well as magnetic and electric fields. In this work, we explore broadband magnetometry using a femtosecond laser-written waveguide hosting a high density of NV centres in diamond [1]. The waveguide simplifies the collection of NV photoluminescence, allowing for fibre integrated high sensitivity broadband magnetic field detection. To date, we have achieved a magnetometry sensitivity of approximately 70 nT/ \sqrt{Hz} while operating at low excitation power, with a clear route to picoTesla sensitivity and below [2]. This approach paves the way for scalable, chip-integrated quantum sensors with applications in bioimaging, material science, and fundamental physics.

Acknowledgements

We acknowledge financial support from EPSRC EP/T017813/1 and EU's H2020 MSCA-ITN LasIonDef (GA-No.956387), and the LPDP Endowment Fund.

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[2] Guo et al, arXiv:2502.02478v1, (2025)

Scalable two-dimensional semiconductors: From photo-gating to deep UV optoelectronics

<u>Benjamin Dewes</u>¹, Nathan D. Cottam¹, Mustaqeem Shiffa¹, Jonathan Bradford¹, Tin S. Cheng¹, Sergei V. Novikov¹, Christopher J. Mellor¹, Oleg Makarovskiy¹, Kazi Rahman¹, James N. O'Shea¹, Peter H. Beton¹, Teresa Ben², David González², Samuel Lara-Avila³, Jordan Harknett⁴, Mark T. Greenaway⁴, Amalia Patanè¹

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2D Materials and Toplogical Devices, June 24, 2025, 14:15 - 16:05

Two-dimensional semiconductors (2SEM) can advance modern science and technologies. However, transforming the semiconductor landscape requires high-quality materials with welldefined electronic properties, which are still difficult to control and scale. Here, these challenges are addressed by integration of growth, scanning probe microscopy and electron spectroscopy of 2SEM in ultra-high vacuum. We use a bespoke facility (EPI2SEM) for EPitaxial growth and In-situ analysis of 2SEM¹. A centrosymmetric polymorph (D3d) of the 2SEM gallium selenide (GaSe) is obtained by epitaxy on sapphire² and graphene/SiC³. Atomically thin layers of GaSe align in the layer plane with graphene with an electronic band structure and electric field dipole at the interface with graphene that are tuneable by the layer thickness.

Epitaxial GaSe represents a scalable building block for nanoelectronics. We present two proof of concept devices. In the first device, the electric dipole at the interface of monolayer GaSe and graphene is very sensitive to photogenerated charges in GaSe. The indirect nature of the bandgap of GaSe and the heavy hole masses can retard band-to-band recombination and facilitate an accumulation of positive charge in GaSe, acting as a photogate for graphene. In the second, GaSe provides a platform for scalable photodetectors. Optical anisotropy and resonant absorption of GaSe and its oxide (Ga₂O₃) in the deep-UV are exploited for photon sensing in the technological UV-C spectral range⁴.

¹YouTube links: http://youtu.be/mtXWhM0s9D4, http://youtu.be/GHCxEDMh3R0 ²M. Shiffa et al., Small 2024, 20, 2305865. ³J. Bradford et al., Small 2024, 20, 2404809.

⁴N. Cottam et al. submitted to ACS Photonics 2025.

Theory of free fermions dynamics under partial post-selected monitoring

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Non-equilibrium, June 26, 2025, 10:30 - 12:50

Monitoring many-body quantum systems can stabilise new out-of-equilibrium steady states with different many-body quantum orders and associated Measurement-induced Phase Transitions (MiPTs) stemming from the interplay between measurements and unitary dynamics. When the detector readout is post-selected to match a given value, the dynamics is generated by a non-Hermitian Hamiltonian with MiPTs characterized by different universal features. Here, we derive a partial post-selected stochastic Schroedinger equation based on a microscopic description of continuous weak measurement. This formalism connects the monitored and post-selected dynamics to a broader family of stochastic evolution. We apply the formalism to a chain of free fermions subject to partial post-selected monitoring of local fermion parities. Within a 2-replica approach, we obtained an effective bosonized Hamiltonian in the strong post-selected limit. Using a renormalization group analysis, we find that the universality of the non-Hermitian MiPT is stable against a finite (weak) amount of stochasticity. We further show that the passage to the monitored universality occurs abruptly at finite partial post-selection, which we confirm from the numerical finite size scaling of the MiPT. Our approach establishes a way to study MiPTs for arbitrary subsets of quantum trajectories and provides a potential route to tackle the experimental post-selected problem.

A Magnon Band Analysis of GdRu2Si2 in the Field-Polarised State

<u>Dr. George Wood</u>^{1,2}, Ross Stewart¹, Daniel Mayoh², Joseph Paddison³, Juba Bouaziz⁴, Siobhan Tobin^{5,6}, Oleg Petrenko², Martin Lees², Pascal Manuel¹, Julie Staunton², Geetha Balakrishnan²

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Magnetism, June 24, 2025, 10:30 - 12:50

Understanding the formation of skyrmions in centrosymmetric materials is a problem of fundamental and technological interest. $GdRu_2Si_2$ is a candidate material which hosts a variety of multi-Q magnetic phases, including in zero-field [1]. Here, inelastic neutron scattering is used to measure the spin excitations in the field-polarized phase of $GdRu_2Si_2$. Linear spin wave theory and a method of interaction invariant path analysis are used to derive a Hamiltonian accounting for the spectra. The Hamiltonian, dominated by bilinear (Ruderman-Kittel-Kasuya-Yosida) Heisenberg exchange, compares favorably to ab initio calculations. Dipolar interactions are a secondary energy scale to consider, with J_dip $\sim 0.05J_RKKY$. However, it is shown that in the field polarized phase the dipolar interactions 'self screen' so that their effect is largely suppressed. No specific evidence for higher-order exchange is found. These aspects are discussed in the context of the lower field multi-Q states and the anisotropy of the system.

[1] G. D. A. Wood et al., Phys. Rev. B 107, L180402 (2023)

[2] G. D. A. Wood et al., (Accepted 2025: npj Quantum Materials) arXiv:2501.01201

The folded pseudochiral Fermi surface of charge density wave material 4Hb-TaSe2

<u>Mugerabe Zerabza</u>¹, Simon Crampin¹, Yu Zhang², Emma Springate², Fabio Boschini³, Nicolas Gauthier³, Niccolò Mignani⁴, Ettore Carpene⁴, Matthew Watson⁵, Enrico Da Como¹ ¹Department of Physics and Centre for Nanoscience and Nanotechnology (CNAN), University of Bath, United Kingdom, ²Central Laser Facility, Research Complex at Harwell, STFC Rutherford Appleton Laboratory, United Kingdom, ³Institut national de la recherche scientifique, Canada, ⁴IFN-CNR, Dipartimento di Fisica, Politecnico di Milano, Italy, ⁵Diamond Light Source Ltd, Harwell Science and Innovation Campus, United Kingdom

2D and 1D Materials, June 26, 2025, 14:15 - 16:05

The tantalum dichalcogenide family of layered materials (TaX₂; X = S. Se) is known to exhibit some unique properties such as Mott insulator behaviour, superconductivity and charge density wave instabilities. Among the different crystal structures, the 4Hb has attracted a lot of attention recently. This is because of the proximity between the Mott-CDW physics in the T layers and superconductivity in the H (1,2). The T-layers exhibit a known Star-of-David superlattice that supports a $\sqrt{13}$ $\times \sqrt{13}$ charge density wave, intercalated by metallic H-layers. Using angle-resolved photoemission spectroscopy (ARPES), we show a star-shaped Fermi surface resulting from the reconstruction of the Brillouin zone. The system allows for band hybridisation, which modulates the overall electronic structure and is notable due to the lack of a band gap at the Fermi level, unlike what has been observed in isolated monolayers of 1T-TaSe₂ (3). Due to the breaking of in-plane mirror symmetry resulting from folded bands in the CDW state, the Fermi surface is described to be pseudochiral, which could be relevant for understanding correlated electron phases in T-H heterostructures (1, 2). Additionally, we explored the dynamics of the band structure. Laser excitation in the hundred femtoseconds regime causes oscillations in the band dispersion, which have a dominant frequency of ~2.2 THz, corresponding to the amplitude mode of the CDW.

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Rhombohedral graphite junctions as physical realisations of topological defects in the Su-Schrieffer-Heeger model

Luke Soneji¹, Simon Crampin¹, <u>Marcin Mucha-Kruczynski¹</u> ¹University Of Bath, United Kingdom

2D and Topological Physics, June 27, 2025, 10:30 - 12:00

The topological properties of quasiparticle dispersions provide a distinct way of categorizing phases of matter and underpin the notions of the topological insulator and topologically protected edge states: important design principles across various areas of physics, including solid state or soft matter physics as well as photonics. We consider electronic properties of interfaces between rhombohedral graphite semi-infinite half-crystals which we show can be understood in terms of coupled Su-Schrieffer-Heeger chains. In particular, we establish that the presence or absence of topologically protected junction states follows from the symmetries of the junctions. Finally, we demonstrate that rhombohedral graphite junctions are a unique system in which the smooth evolution of topological states between the topologically trivial and nontrivial phases can be tracked by sliding one of the crystals with respect to the other.

Enhancing the thermoelectric performance of molecular layers via $\pi\text{-}\pi$ stacking.

James Newson¹, Harry Redfern¹, Jake Seward¹, Samuel Harley¹, Benjamin Robinson¹, Samuel P. Jarvis¹

¹Lancaster University, United Kingdom

Thin-Films, June 25, 2025, 14:15 - 16:05

It is estimated that 52% of global energy produced is lost during the conversion from primary energy carriers to final use due to waste heat [1]. Thermoelectric materials are therefore an attractive method of recycling this waste heat into electricity, reducing the amount of energy that needs to be produced overall. Current high performing inorganic thermoelectric materials are typically made using scarce materials [2] and often require high temperatures to efficiently recycle waste heat. In contrast, organic materials have been shown to operate at much lower temperature gradients more suitable for harvesting waste heat, and can be made with nontoxic, sustainable materials [3]. The trade-off, however, is a reduction in performance compared to the leading materials.

Recently we have shown that π - π stacking can enhance the Seebeck coefficient of layers of zinc tetraphenylporphyrin [4], whilst also reducing the phonon transport and therefore thermal conductivity of the layer. Here, we move beyond this study, reporting measurements on a series of tetraphenylporphyrin (TPP), phthalocyanine (Pc) and naphthalocyanine (NPc) derivatives. Growth of molecular mono- and multi-layers via thermal sublimation is characterised using XPS and SPM. We then compare Seebeck coefficients and electrical conductivity to investigate how varying π - π overlap and also metal center atoms can lead to enhancement of thermoelectric properties.

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On-surface bottom-up growth of graphene nanoribbons on SiO2

<u>Elisabeth Bancroft</u>¹, Alessio Quadrelli¹, David Buceta², Manuel Arturo Lopez-Quintela², Shi-Xia Liu², Samuel Jarvis¹ ¹Lancaster University, United Kingdom, ²University of Santiago de Compostela, Spain, ³University of Bern, Switzerland

Nanoscale and 2D, June 24, 2025, 10:30 - 12:50

Graphene nanoribbons (GNRs) are attractive for use in molecular electronic devices as they exhibit exceptionally high mobility and on/off ratios [1] that are structure-dependent [2]. To maintain these properties, GNRs must be defect free and atomically precise making a bottom-up method preferable. This requires surface-assisted reactions between monomers, requiring catalytically active substrates such as Au(111). This creates challenges when transferring GNRs to CMOS compatible substrates such as SiO2, where transfer methods such as stamping remain a stubbornly low-yield process.

Here, we describe results demonstrating an alternative route to solve this challenge by fabricating GNRs directly onto SiO2. We use the precursor monomer 10,10'-dibromo-9,9'-bianthryl (DBBA) to fabricate GNRs, the growth of which is monitored in situ using temperature-programmed X-ray photoelectron spectroscopy (TP-XPS). We show that atomic quantum clusters (AQCs) – small clusters of metal atoms, 5 atoms in size and exhibiting a molecule-like band gap [3,4] – can be used to activate surface polymerisation of DBBA. In particular we show that Ag5OX AQCs can be deposited onto SiO2 substrates via spin-coating under controlled conditions. A combination of TP-XPS, SPM, and Raman spectroscopy is then used to study the effect of Ag5OX on the surface-assisted reaction of DBBA on SiO2.

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Semiclassical Trace Formula for Lieb-Liniger Model

David Martin¹, Remy Dubertrand¹ ¹Northumbria University, United Kingdom

Statistical and Nonlinear, June 25, 2025, 10:30 - 12:50

In quantum chaos, an important tool to study the correspondence between a quantum system and its classical limit is the trace formula. This relates the energy density of a quantum model to the properties of the periodic solution

of its classical limit. Here we apply the trace formula to the Lieb-Liniger model for a finite number of particles. This model has played a central role in mathematical physics and, we aim to show, is particularly relevant for studying classical/quantum correspondence. The model deals with N 1-Dimensional Bose particles trapped in a box, interacting via a two-body potential chosen as the Dirac delta "function". We consider the repulsive interaction strength regime in our derivations.

The original treatment by Lieb and Liniger uses the Bethe ansatz to find the energy spectrum and the corresponding eigenstates. The oscillating part of the trace formula will relate the quantum energy spectrum to the classical periodic trajectories. We test our trace formula in two ways. First by solving numerically the Bethe equations for a given N, computing a long sequence of levels to get their density and comparing with the asymptotic Weyl's law. Then comparing the obtained density with a sum over the periodic classical solutions. We also discuss the spectral statistics for the model.

Investigation of correlation effects mediated by impurity in a onedimensional quantum wire via dc source-drain bias spectroscopy

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Nanoscale and 2D, June 24, 2025, 10:30 - 12:50

The electrostatic confinement of one-dimensional (1D) channels using split-gate techniques enables exploration of novel quantum effects. Varying the channel width using split gates shifts the Fermi level through 1D subbands, resulting in conductance quantisation in units of 2e^2/h, as described by the Landauer formalism for noninteracting electrons. However, electronelectron interactions give rise to additional phenomena such as the 0.7 anomaly, fractional quantisation in zero magnetic field and 1D Wigner lattice formation [1,2]. The effect of disorder on these correlation effects remains an open question. Here, we present electron transport in a moderately disordered 1D quantum wire fabricated using a GaAs/AlGaAs heterostructure with split and top gates. Using dc source-drain bias spectroscopy, we examine nonlinear transport under varying electron concentrations in zero and 10 T in-plane field at 45 mK. Our results reveal the disorder-modified correlation effects. We identify the emergence of two conductance states below e²/h at large dc bias, which become more pronounced together with 0.7-like features in higher order subbands as electron concentration decreases, indicating strong correlation effects. The weak Zeeman splitting in the ground state, despite a large in-plane magnetic field, suggests that disorder-driven correlations dominate transport in the low-density regime.

The work is funded by the United Kingdom Research and Innovation Future Leaders Fellowship, the Engineering and Physical Sciences Research Council, the Royal Society and the Science and Technology Facilities Council (STFC).

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- [2] S. Ho et al., Phys. Rev. Lett. 121, 106801 (2018).

Manipulating quantum states in multi-gated 1D systems

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Nanoscale and 2D, June 24, 2025, 10:30 - 12:50

One-dimensional systems confined by lateral surface gates traditionally exhibit integer quantization in 2e2/h. More rarely, fractional states have also been observed in these onedimensional systems by employing the modulation of carrier density and confinement potentials [1,2]. These systems often feature a simple three-gate geometry, consisting of two gates for confining electrons and a third top gate for carrier concentration modulation. Despite the simplicity of these systems, the underlying physics is deceptively complex, with the origins of phenomena such as the 0.7 structure and the recently observed fractional conductance plateaus remaining a challenge [1]. For potential integration into quantum computation schemes, an understanding of the underlying physics of these systems in both simple and complex geometries is essential.

In this work, we present experimental results on the observations of a fractional state e2/h formed within a complex gate geometry utilising a multi-gate system. Measurements take place through lateral confinement of a 90nm deep 2D electron gas (2DEG) formed through a GaAs/AlGaAs heterostructure. We observe their absence and onset once the system is pushed from symmetric to highly asymmetric confinement. The wires enter a coupled transport regime, that's cumulative effects displaying the fractional states predominantly at e2/h. We investigate both the cumulative effects of transport through the system, and their individual contributions.

The work is funded by the UKRI Future Leaders Fellowship, EPSRC, STFC and the Royal Society.

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[1] Kumar et al, Phys Rev Lett 2019;122(8):086803; Appl Phys Lett; 2021;119;110502.

[2] Montagu et al, Appl Phys Express (2025): 18 015002.

Quantised conductance in one-dimensional quantum wires

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Nanoscale and 2D, June 24, 2025, 10:30 - 12:50

Electron transport in one-dimensional (1D) quantum wires is a subject of significant interest in both physics and engineering. The transport in the wires becomes ballistic when the channel length is comparable to the mean free path of electrons, leading to the quantised conductance of N(2e^2/h), where N is an integer, and the factor of two comes from the spin degeneracy, which can be lifted using an in-plane magnetic field. The spin polarised plateau at e2/h has been reported in InAs-based quantum point contacts with an asymmetric confinement [1,2]. In a GaAs quantum wire, the e2/h plateau has recently been reported for a back-gated split gate device, attributing exchange and correlation phenomena to the observed effect [2]. Here, we report experimental results of transport in 1D quantum wires fabricated using a quantum well formed in a GaAs/AlGaAs heterostructure. The 1D quantum wire is formed using a pair of split gates, and an additional top gate to control the confinement and carrier density within the 1D channel. We show the observation of the e2/h plateau under both asymmetric and symmetric confinement potentials, and investigate the observed feature using source-drain bias spectroscopy, in-plane and perpendicular magnetic fields and varying temperature conditions.

The work is funded by the United Kingdom Research and Innovation Future Leaders Fellowship, the Engineering and Physical Sciences Research Council, the Royal Society and the Science and Technology Facilities Council (STFC).

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- [2] Montagu et al. Applied Physics Express (2025): 18 015002.

Extracting Topological Information from the Interface Green's Function

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Strongly Correlated Materials, June 24, 2025, 14:15 - 16:05

In condensed matter physics, topology is a field concerned with phases of gapped systems that re-main robust under deformations that preserve the gap and protecting symmetries. However, reliably accessing topological information of a material in an experiment remains a challenge. Green's func-tions may provide key insights for this purpose. They serve as a powerful theoretical tool for charac-terizing quantum many-body dynamics while remaining experimentally accessible through tech-niques like scanning tunnelling microscopy (STM) and angle-resolved photoemission spectroscopy (ARPES).

Here, we present an adaptation of an interface Green's function formalism [1], which allows us to express all surface properties only in terms of the bulk quantities, incorporating the physics of the bulk-boundary correspondence. We then apply this approach to propose an STM-based edge qua-siparticle interference (eQPI) experiment and show, for the case of a topological p+ip superconduc-tor how this measurement can be used to explore experimental signatures of different topological phases.

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What a drag: computational investigation of highly sluggish diffusion in Fe-Ni alloys

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Computational Physics, June 25, 2025, 10:30 - 12:50

In this work, we present a density functional theory (DFT) study of diffusion pathways in nearequiatomic, ferromagnetic Fe-Ni alloys. Our calculations provide insight into why Ni diffusion in this system is particularly slow—approximately 20 times slower than Fe. This sluggish diffusion directly affects the formation of the atomically ordered L10 FeNi phase, tetrataenite, a meteoritic mineral which is being explored as a sustainable permanent magnet [2]. Experimental studies have reported this anomalously slow diffusion behavior [1], a finding now corroborated by our first-principles calculations.

To quantify the diffusion barriers, we perform nudged elastic band (NEB) calculations, evaluating nearly 200 individual barriers. On average, Ni exhibits a significantly higher barrier than Fe, contributing to its reduced mobility. To further understand this behavior, we analyze the underlying electronic structure of these barriers. This deeper insight into the electronic-scale mechanisms governing diffusion enhances our understanding of the kinetics of the A1/L10 disorder-order transformation. With this knowledge, we aim to identify strategies to accelerate the ordering process, potentially improving the viability of tetrataenite as a permanent magnet.

Acknowledgments: This work is supported by US DoE Award DE SC0022168, US NSF Award 2118164 and UK EPSRC Grant EP/W021331/1.

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An emerging security technology: using quantum dots to produce Optical Physically Unclonable Functions

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M4QN I, June 25, 2025, 10:30 - 12:50

Rapid advances in nanostructure design and optical characterisation have opened unprecedented opportunities in hardware security. Optical physically unclonable functions (O-PUFs) exploit random manufacturing variations to generate unique, tamper-resistant identifiers, making them prime candidates for next-generation security primitives. Since Pappu et al. (2002) introduced O-PUFs, implementations have spanned diverse materials from quantum dots (QDs) to silk fibers. Here we harness CuInS/ZnS QDs to develop O-PUFs with distinctive optical signa-tures—a novel approach in the field.

A critical barrier to O-PUF commercialisation has been the lack of standardised evaluation metrics and protocols. We address this challenge by introducing the first unified, backwardcompatible evaluation framework for standardised O-PUF testing and benchmarking. We also provide an open-source Python toolkit, lowering entry barriers and accelerating adoption as O-PUF technology moves toward real-world applications. In refining key metrics from the literature, we identify and adapt those most suitable for image-based O-PUF data, ensuring fair comparisons across implementations. Beyond standardisation, we explore secondary security tests tailored to QD-based O-PUFs, offering an additional authentication layer that leverages the unique properties of these quantum dots. By integrating structured nanomaterials with advanced optical analysis, our approach paves the way for robust anti-counterfeiting measures. This work reinforces O-PUFs as a key enabler of secure, cost-effective optical security technologies. Importantly, we invite collaboration with other research groups in quantum dots and emerging quantum materials to broaden the impact of this effort.

Magnetically-controlled Vortex Dynamics in a Ferromagnetic Superconductor

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Unconventional Superconductivity, June 26, 2025, 10:30 - 12:50

Superconductivity in the iron-based superconductor $EuFe_2(As_{0.79}P_{0.21})_2$ (Tc $\simeq 25$ K) exhibits full coexistence with a uniaxial ferromagnetic state below the Eu2+ moment ordering temperature (TFM = 19 K). MFM imaging has revealed two distinct stripe ferromagnetic domain structures; the Domain Meissner State just below TFM where the domain period is renormalized by Meissner screening currents near domain walls, and the Domain Vortex State characterised by the spontaneous nucleation of vortices and antivortices at lower temperatures. To explore the vortex dynamics in these regimes, we have performed bulk magnetometry, magnetic relaxation and MFM measurements. We find that the magnetic irreversibility is strongly dependent on the presence of both magnetic and superconducting orders. Just below TFM we observe a pronounced peak in the creep activation energy while in the same regime MFM measurements reveal extremely closely spaced (separation w $\ll \lambda$) vortex clusters. We attribute these observations to the formation of vortex polarons arising from the local perturbation of the stripe domain structure by the vortex magnetic fields and develop a qualitative theory for this. Our work suggests new routes for the magnetic enhancement of vortex pinning with important potential applications in high-current conductors.

Resolving the Fermi surface and detection of anisotropic vortex pinning in FeSe

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Unconventional Superconductivity II, June 26, 2025, 14:15 - 16:05

Among all Fe-based superconductors, FeSe has the simplest structure and yet has proven to host some of the richest and most tunable physics. Evidence exists for nematic quantum criticality as well as topological superconductivity, for high temperature superconductivity in monolayers, under pressure or with electron doping, and for strange-metal behaviour. FeSe has also drawn interest due to its unique nematic without magnetic order and low carrier density promoting correlation effects. Here, we present two new results on FeSe. First, we perform detailed c-axis angle dependent magnetoresistance (ADMR) and Shubnikov-de Haas measurements. Both measurements individually allow us to resolve the bulk Fermi surface of FeSe. Uncertainty about the Fermi surface has hindered our understanding of FeSe for the last decade and a resolution is expected to aid theoretical efforts to model the superconductivity and high tunability of FeSe. Secondly, we extend our ADMR measurements into the vortex liquid state of FeSe and observe strongly anisotropic vortex pinning as a function of in-plane magnetic field angle. This result highlights the strong vortex pinning by twin boundaries even in partially detwinned FeSe and reveals furthermore unexpected vortex pinning 45 degrees away from the twin boundaries, which at present is poorly understood. Together, these results enable more control and a deeper understanding of FeSe to harness its tunability and rich physics.

Understanding quantum materials through chemical bonding models

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Superconductivity I (IOP SC Group), June 24, 2025, 10:30 - 12:50

Superconductors and topological materials are two classes of quantum electronic material with wide-ranging applications in next-generation technologies if their critical properties can be realised under practical device operating conditions. For accelerated discovery of new quantum materials, chemically intuitive bonding models for inorganic solids with exotic electronic properties are required. In this talk I will illustrate this approach with two case studies, one on the high-pressure hydrides LaH10 and EuH9,and one on the topological crystalline insulator SrAg4Sb2 and EuAg4Sb2. Density functional theory calculations can simplify the interpretation of complex electronic phenomena in solids through properties including atomic charges, pairwise bond strengths, and orbital-resolved band structures. In the hydrides we have demystified the elegant, symmetrical hydrogen sublattices by identifying the ionic and covalent interactions that underpin them.[1] In the topological insulators we have characterized the band inversion in terms of Ag-Ag bonding interactions,[2] verifying our calculations with quantum oscillation measurements,[3,4] and I will show how this guides our ongoing search for observable topological phenomena.

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Investigation of magnetic field-induced quantum transport phenomena in tungsten ditelluride

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2D Materials, June 25, 2025, 14:15 - 16:05

The Seebeck effect describes the thermo-electric phenomenon where a voltage is induced due to an applied thermal gradient. This effect is quantified by the Seebeck coefficient. Tungsten ditelluride in the 1T' phase (WTe2) has particularly interesting thermo-electric properties including a large unsaturated magnetoresistance [1] and a change in polarity of the Seebeck coefficient with increasing temperature [2]. These phenomena are attributed to the unique electronic properties of WTe2: it is a topological Weyl semimetal with electron and hole pockets at the Fermi energy [3].

Here, we use the Kubo formalism to provide an in-depth analysis of the thermo-electric properties of WTe2 in strong, quantising magnetic fields. To explain the experimental measurements, we tune the effective masses, band offsets and carrier concentration of a 4-band model for WTe2 with impurity scattering (inter- and intra-band scattering) included via the self-consistent Born approximation. Our analysis of the complex Shubnikov de Haas oscillations explains the temperature dependence of the Seebeck coefficient, in particular its change in polarity [2]; reveals the importance of inter-valley scattering; and finds minimal influence from the Zeeman effect. Our results will be useful for developing the thermo-electric applications of WTe2 (e.g. energy recapture from thermal losses) and can be extended to understand magneto-oscillations in other charge-compensated semi-metallic systems.

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Probing moiré electronic structures through quasiparticle interference

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2D Materials, June 25, 2025, 14:15 - 16:05

Moiré lattices are a general feature of bilayer structures, where an additional periodic superstructure is generated by either lattice mismatch or from a twist angle. They have been shown to stabilise new ground states, including unconventional superconductivity and Mott insulating phases, attributed to strong electron correlations. However, controlling these interactions requires a detailed understanding of the low energy electronic structure which is lacking so far. Probing the electronic structure is challenging due to sample inhomogeneity, the low characteristic energy scales involved and small sample sizes. Through quasiparticle interference (QPI) imaging, scanning tunneling microscopy (STM) can overcome many of these challenges but requires detailed modelling to extract the k-space electronic structure. Here, we present realistic calculations of QPI in twisted bilayer structures, which accounts for the effect of the long range Moiré lattice on the electronic structure as well as it's interaction at a defect. These calculations reveal that while the moiré supercell significantly reduces the size of the Brillouin zone, the QPI scattering vectors retain characteristics of the individual monolayers with distinct perturbations from the twisted geometry that can be directly linked back to the electronic structure. The procedure introduced here provides a general framework to use QPI to determine the low energy electronic structure in moiré lattice systems.

Changing the Seebeck Coefficient Polarity of a Self-Assembled Monolayer by Surface Interaction

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Thin-Films, June 25, 2025, 14:15 - 16:05

Here we report recent experiments using advanced scanning probe approaches to study the thermoelectric properties of highly ordered molecular monolayers in ambient conditions. The observation of room temperature quantum interference (QI) effects in single molecules has opened up new possibilities for molecular electronics and thermoelectric materials. Recent reports demonstrate that single-molecule QI effects can be translated into self-assembled monolayers (SAMs), which retain excellent thermoelectric properties, even with the absence of long-range order within the layers. Molecular design plays a crucial part in the thermoelectric performance of a SAM, however we demonstrate how the formation of a SAM and the molecule-surface interaction can also be of critical importance, to the point of changing not only the magnitude, but also the polarity of measured Seebeck.

SAMs of Oligo(phenylene ethynylene) molecules (OPE3) designed with alkyl-alkyne side chains were grown on template-stripped gold and subsequently analysed by XPS, AFM, conductive AFM, and a bespoke application module for Seebeck measurements. We show that whilst the fused molecule 3 exhibits an expected negative Seebeck coefficient, molecules 1 and 2 were measured to have positive Seebeck. We show that this is driven by the alkyne "arms" of molecules 1 and 2 interacting with the gold, which through simulation we show causes the HOMO-LUMO peaks to shift in such a way relative to the fermi energy of the electrode that the polarity of the Seebeck coefficient changes.

Quantum Spectral Sampling for Quantum Link Models

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Strongly Correlated Electron Systems, June 26, 2025, 14:15 - 16:05

Quantum link models (QLMs) have gained attention in recent years, as a framework for discretising gauge theories which is especially

suited to quantum computation approaches, and which often exhibit exotic phases of matter, allowing one to address dynamical

properties related to quantum many-body scarring and Hilbert-space fragmentation which are otherwise difficult to study.

We choose to focus on the SO(3) QLM because of qualitative properties it is known to share with QCD, including fermionic baryon bound states, and spontaneous chiral symmetry breaking (in (1+1)d). More recently, a subset of us have studied the matter-free SO(3)

QLM in (2+1)d using quantum algorithms to demonstrate spontaneous

symmetry breaking. In recent work to be reviewed in this talk, we have constructed the gaugeinvariant state space for the SO(3) QLM in (2+1)d with dynamical fermions, and obtained ED results which demonstrate spontaneous symmetry breaking and a non-trivial phase space for a single plaquette.

In this talk, we demonstrate how a recently proposed quantum algorithm for whole-spectrum sampling, which takes advantage of maximally-mixed states, can be applied to QLMs to great effect. Such methods have general applicability across the domain of quantum simulation for physical systems, and in presenting an algorithm which may be unfamiliar to many practitioners, we will emphasize several distinct types of physical data which can be efficiently extracted by such a technique. We will compare in detail with properties of analogous classical spectroscopy algorithms, and examine how both physics at nonzero chemical-potential and finite temperatures can be obtained from this method.

A Low Energy uSR study of proximity superconductivity in a high spin orbit coupling semiconductor 2DEG

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Spin-Orbit, June 24, 2025, 14:15 - 16:05

Proximity induced superconductivity in high spin orbit coupling semiconductors is thought to exhibit a mixed s-wave and $p_x\pm ip_y$ state [1]. In appropriate device geometries, such a system should host Majorana Zero Modes which can form the basis of a qubit with inherent protection from decoherence [2]. However, claims of the successful realisation of such a topological state remain under debate [2] [3]. Muon Spin Spectroscopy (μ SR) offers an alternative experimental insight into these systems. By measuring the local field within a sample, μ SR can detect signatures of non s-wave components of superconductivity. This has previously measured odd frequency components of proximity superconductivity induced in a topological insulator [4].

We present low energy μ SR measurements of an InSb 2DEG heterostructure with a surface Pb thin film. We observe evidence of magnetic field screening extending ~10s of μ m from the Pb/InSb interface. We also observe that screening profile is altered by an increasing external magnetic field, a potential indicator of induced p_x±ip_y pairing. Additionally, we present supporting electrical measurements on Nb thin film/InSb devices. Our results hope to highlight the unique insight μ SR can offer into proximity induced superconducting systems.

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Topological Singularities in Twisted Kagome Bilayers

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2D Materials, June 25, 2025, 14:15 - 16:05

Quantum geometry and strong correlations yield a plethora of emergent phases in materials heavily influenced by the details of interactions. The Kagome lattice is a natural playground for probing strong correlations, hosting an exactly flat band and van Hove singularities (VHSs). By creating a Kagome bilayer, we explore the possibility of band engineering through methods that have proven invaluable in van der Waals heterostructures [1-3]. Of particular interest are higher-order VHSs (HOVHSs) yielding a power-law divergence of the density of states (DOS) [4].

In this talk, we analyse the symmetries of twisted bilayer Kagome (TBK) to determine which HOVHSs it may host [5]. We demonstrate how HOVHSs with two-, three- and six-fold rotational symmetry can be achieved in TBK using dimerisation, complex next-nearest-neighbour tunnelling, and out-of-plane electric fields as tuning parameters. We observe a wide range of parameters yielding HOVHSs exhibiting the expected DOS signatures. Using complex next-nearest-neighbour tunnelling, we establish a zoo of topological HOVHSs where the interplay of topology and interactions are expected to be central in determining the emergent phase [6].

Acknowledgements

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[6] Perkins et al., submitted (2025)

Quasiparticle Interference of Spin-Triplet Superconductors: Application to UTe2

Hans Christiansen¹, Max Geier², Brian M. Andersen¹, Peter J. Hirschfeld³, <u>Andreas Kreisel¹</u> ¹University of Copenhagen, Denmark, ²Massachusetts Institute of Technology, USA, ³University of Florida, USA

Unconventional Superconductivity, June 26, 2025, 10:30 - 12:50

Quasiparticle interference (QPI) obtained from scanning tunneling microscopy (STM) is a powerful method to help extract the pairing symmetry of unconventional superconductors. It turns out that triplet superconductors behave qualitatively different than singlet superconductors in QPI. This is due to the vector nature of the d-vector describing the pairing state in spin space such that the relative orientation of this vector of the quasiparticle states contributing to the scattering process deduces the expected scattering amplitude. We examine general properties of QPI of triplet superconductors in the bulk and on the topological surface bound states. As a concrete example we apply the theory to a model specific to UTe2, a promising candidate material hosting intrinsic spin-triplet superconductivity. To this end, we start with a multiband model of the electronic structure and an ansatz for the superconducting order parameter of the two candidate Cooper pair instabilities B2u and B3u. Examining the surface Dirac states and flat bands on the experimentally relevant (0-11) surface, we find unique signatures that help pinpointing the pairing symmetry channel of UTe2.


Figure 1: Quasiparticle interference of triplet superconductors (a) Visualization of the d-vector (black arrows) of a B_{3a} triplet state along a path (blue line) of high density of states. There exist scattering processes with all possible relative angles between the d-vectors; three of them are shown for $\theta=0, \pi/2, \pi$ (red and purple arrows). (b) Fermi surface of UTe₂ (blue: Te states / red: U states) with the nodal points of the superconducting order parameter (red, eyan dots) marked. (c) Spectral function A(k, ω) of the bulk superconductor (blue) and the surface state (green) which exhibits Dirac states (green circles) (d) QPI of the bulk with characteristic scattering vectors from nodal points and (e) surface QPI with dominant scattering between the Dirac surface states centered at the time-reversal invariant points.

Hans Christiansen, Max Geier, Brian M. Andersen, Andreas Kreisel, arXiv:2503.11603
 Hans Christiansen, Brian M. Andersen, P. J. Hirschfeld, Andreas Kreisel, arXiv:2505.01404

Universal transport at Lifshitz metal-insulator transitions in two dimensions

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2D and 1D Materials, June 26, 2025, 14:15 - 16:05

Graphene, transition-metal dichalcogenides, and their twisted heterostructures provide a new platform to study 2D physics with unprecedented precision. Recently, a band-tuned metalinsulator transition (MIT) was experimentally realized in a field-tuned MoTe₂/WSe₂ moiré bilayer. For high temperatures T and chemical potentials µ far from the transition point, electronic conduction in this system is ballistic and the resistance R(T) verifies a simple oneparameter scaling relation. Here, we explore the limits of this semi-classical behaviour and study the ill-understood quantum regime beyond, where scaling breaks down. We derive an analytical formula for the simplest Feynman diagram of the linear response conductivity $\sigma =$ 1/R of a parabolic band endowed with a finite lifetime. Our formula shows excellent agreement for the MoTe₂/WSe₂ bilayer experiment as it captures the guantum effects responsible for breaking the one-parameter scaling. We go on to discuss a fascinating prediction of our model: The resistance at the quantum-critical band-tuned Lifshitz point ($\mu = T = 0$) has the universal value, RL = $(2\pi h)/e^2$, per degree of freedom. This value is found to be compatible with the available experiment and should apply to any band-tuned MIT in 2D. Finally, we hypothesise that RL provides an upper bound for the critical resistance at a 2D Anderson transition and that a critical resistance greater than RL is a sufficient (but not necessary) condition for an MIT to be predominantly driven by strong correlations. Reference: arXiv:2501.17616

Improving the stability of thin films for molecular electronics through on-surface cross-linking.

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Thin-Films, June 25, 2025, 14:15 - 16:05

Thermoelectric molecular thin films offer a promising approach for converting low-grade waste heat into electrical energy. Unlike conventional thermoelectric generators, these films utilize a perpendicular heat gradient, making them well-suited for seamless integration into various devices. Oligo(phenylene ethynylene) (OPE) molecules are particularly promising for thermoelectric applications due to their π -conjugated structure, which enables efficient electron transport and enhances electrical conductivity due to room temperature quantum interference effects [ref]. Here we propose to further enhance their thermoelectric performance using alkyl chains to facilitate crosslinking between molecules, designed to not only improve molecular stability and longevity, but also suppress phonon modes, thereby reducing thermal conductivity and improving overall efficiency.

We investigate self-assembled monolayers (SAMs) of OPE molecules on gold-coated mica substrates, focusing on branched arylene ethynylene-based molecules (OPE3) with pendant arm groups. SAMs are prepared by solution self-assembly, followed by thermal annealing under UHV conditions with in situ X-ray photoelectron spectroscopy (XPS). XPS and atomic force microscopy (AFM) measurements confirm the chemical changes and increases in mechanical stability expected through crosslinking. These results, alongside measurements of molecular conductance and Seebeck, highlight the impact of molecular design and polymerisation techniques on the durability and efficiency of organic thermoelectric materials.

Collective Excitations in Altermagnets: A Fermi Liquid Approach

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Magnetism, June 24, 2025, 10:30 - 12:50

Altermagnetism is an emerging class of magnetic materials characterised by compensated antiparallel magnetic order. The altermagnetic band structure breaks time-reversal symmetry and exhibits non-relativistic spin splitting, even in the absence of spin-orbit coupling [1]. Quasi-2D altermagnets, such as Mn\$_5\$Si\$_3\$, which display effectively two-dimensional spin-textured, anisotropic low-energy bands and weak dispersion along the third dimension, are attracting significant attention. The interplay of spin texture, anisotropy, and electronic spin and density in altermagnetic systems suggests that the collective modes in these materials exhibit novel characteristics, distinct from those in conventional metals.

In this talk, I will present a Fermi liquid framework for an altermagnetic system and investigate the associated charge and spin collective excitations [2]. Our numerical results show that the dispersion, lifetime, and spectral weight of these modes can be significantly tuned by varying the propagation direction and the phenomenological Landau parameters characterising interparticle interactions. Our study provides a basic understanding of collective excitations in altermagnets within a specific Fermi liquid framework, which may also have implications for other systems with a nematic Fermi surface.

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Enhancing optoelectronic devices with exciton topology

<u>**Dr Joshua Thompson**</u>¹, Wojciech Jankowski¹, Robert-Jan Slager^{1,2}, Bartomeu Monserrat¹ ¹University Of Cambridge, United Kingdom, ²University of Manchester, United Kingdom

2D Materials and Toplogical Devices, June 24, 2025, 14:15 - 16:05

The properties and performance of many optoelectronic devices, from solar cells to light-based biosensors, depends on the behaviour of excitons, Coulomb-bound electron-hole pairs. Schemes to enhance the transport of these excitons are highly desirable, as transport is often one of the key limiting factors in device performance. Inspired by the topology of electrons, we explore how the topology of excitons in a real organic material system can be induced, depending on a complex interplay between the topology of the underlying electronic states and their interactions [1]. Using a combination of microscopic theory and ab-initio calculations, we provide a blueprint for how the topological phase can be tuned via chemical design. Importantly, we demonstrate that topological excitons undergo significantly enhanced transport compared to their trivial counterparts, across a wide range of time scales and regimes [2]. We explore the impact of exciton topology on the material response to strain, phonons and non-uniform electric fields. Owing to the generality of our findings, our work provides a new, ubiquitous tool through which excitonic properties can be controlled and enhanced, for the betterment of state-of-the-art optoelectronic devices.

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Electronic structure and charge-density wave modulation in monolayer TiSe2

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2D Materials, June 25, 2025, 14:15 - 16:05

Transition metal dichalcogenides are prototypical layered materials known for hosting a variety of quantum phases down to the two-dimensional limit. Among them, $TiSe_2$ is an exemplary case that has been subject of interest for the emergence of a controversial charge-density wave (CDW) state, characterized by an in-plane 2×2 superlattice [1]. This CDW persists down to the single-layer limit [2], and claims of potential chiral CDW and elusive excitonic insulator phases have been proposed [3-6].

In this work, we investigate monolayer TiSe₂ synthesized via molecular-beam epitaxy and characterize its electronic structure using a combination of in-situ angle-resolved photoemission spectroscopy (ARPES) and scanning tunnelling microscopy/spectroscopy (STM/STS). High-resolution ARPES measurements and quasi-particle interference patterns obtained from STM/STS allow us to determine the electronic band structure in both the occupied and unoccupied states. Based on these results, we construct realistic tight-binding models that capture the emergence of a rich spectrum of van Hove singularities in TiSe₂. These models, in turn, enable us to investigate real space modulations of the electronic structure and their connection to the spatial variation of the CDW phases.

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Higher-harmonic superconductivity driven by van Hove singularities in the third-nearest-neighbour square-lattice Hubbard model

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Superconductivity I (IOP SC Group), June 24, 2025, 10:30 - 12:50

The functional renormalization group (FRG) is a powerful theoretical tool for deducing the lowenergy behaviour of a given lattice model. By unbiasedly treating the competition between different ordering instabilities, it can give unprecedented insight into the ground states of strongly correlated itinerant electron systems. Until recent years, applying it to any more than simple models with limited momentum resolution was very computationally expensive; however, this has changed with the advent of truncated-unity FRG [1], which is scalable and can treat arbitrary electronic structures with full momentum resolution.

Using truncated-unity FRG, we study the phase diagram of the 2-D, square-lattice Hubbard model with up to third nearest-neighbour hoppings. Inclusion of a third nearest-neighbour hopping causes the appearance of extra van Hove singularities, which dramatically impact the correlated ground state. We show that higher-harmonic d-wave superconductivity is stabilized, and discuss how the gap structure varies with proximity to nearby phases. We also provide analytic insight into our results using a four-patch parquet-renormalization-group analysis, before concluding with some possible implications for experiment.

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A generalised Haldane map from the matrix product state path integral to the critical theory of the J1-J2 chain

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Frustrated Magnetism and Spin Ice, June 27, 2025, 10:30 - 12:00

We present the results of a theoretical study of the J1-J2 spin-1/2 chain using a path integral constructed over matrix product states (MPS). By virtue of its non-trivial entanglement structure, the MPS ansatz captures the key phases of the model even at a semi-classical, saddle-point level, and, as a variational state, is in good agreement with the field theory obtained by abelian bosonisation.

Going beyond the semi-classical level, we show that the MPS ansatz facilitates a physicallymotivated derivation of the field theory of the critical phase: by carefully taking the continuum limit - a generalisation of the Haldane map - we recover from the MPS path integral a field theory with the correct topological term and emergent SO(4) symmetry, constructively linking the microscopic states and topological field-theoretic structures. Moreover, the dimerisation transition is particularly clear in the MPS formulation - an explicit dimerisation potential becomes relevant, gapping out the magnetic fluctuations.

ARPES-derived anomalous spectral weight across the Fermi surface of the strange metal phase

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Unconventional Superconductivity II, June 26, 2025, 14:15 - 16:05

The strange metal phase in high-Tc cuprates defies conventional metallic behavior, challenging our understanding of electron correlations and quantum criticality. Marked by anomalous transport properties and unconventional scattering, this state has become a central puzzle in condensed matter physics and superconductivity research. A key discrepancy lies at its heart: while angle-resolved photoemission spectroscopy (ARPES) consistently detects a full Fermi surface with a carrier density of n = 1 + p, Hall effect measurements reveal a transition from n = p to n = 1 + p. Reconciling these seemingly conflicting observations is crucial, as doing so could unlock critical insights into how charge carriers evolve during the transition from superconductivity to the strange metal phase, and ultimately shed light on the pairing mechanism driving high-Tc superconductivity.

In this work, we aim to bridge the gap between ARPES and transport measurements. We employ a refined, quantitative ARPES analysis on high-resolution data from single-layer Bi2201 to meticulously map the electronic structure and examine the momentum-dependent response of quasiparticle away from the nodal region. This approach allows us not only to test the limits of ARPES as a probe of single-particle dynamics but also to reveal how collective many-body phenomena, which are central to transport properties, emerge in these experiments. Our results offer a new perspective on the interplay between single-particle excitations and many-body interactions which drive the strange metal phase.

Determination of spin-orbit interaction via nonlinear transport

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Frustrated Magnetism and Spin Ice, June 27, 2025, 10:30 - 12:00

I present a framework for probing spin-orbit interaction (SOI) in low-dimensional semiconductors via nonlinear electrical responses. First, a semiclassical Boltzmann-relaxation-time approach shows that second-harmonic current or voltage measurements in one- and two-dimensional systems yield direct benchmarks of linear and cubic SOI. Second, a Keldysh-Green's-function analysis incorporates interband (quantum-metric and Berry-curvature-dipole) contributions alongside impurity scattering, allowing access to regimes where semiclassical approximations break down and interband couplings become important. Finally, nonlinear Shubnikov-de Haas oscillations in two-dimensional hole gases exhibit distinct behavior depending on whether cubic or linear SOI is dominant, providing a clear fingerprint for separating and quantifying different spin-orbit strengths.

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Time-Reversal Symmetry Protected Transport at Correlated Oxide Interfaces

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Strongly Correlated Electron Systems, June 26, 2025, 14:15 - 16:05

Time-reversal symmetry (TRS) protection is core to topological physics, yet its role in correlated oxides-typically non-topological-remains underexplored. This limit hampers the potential in engineering exotic quantum states by fusing TRS protection and the rich emergent phenomena in the oxide platform. Here, we report evidence of a TRS-protected subband at oxygen vacancy-free LaAI03/SrTiO3 interfaces. This subband causes a low-field quantum oscillation with anomalous characters: exceptionally light electron mass, aperiodicity, susceptibility to magnetic fields and tunability through uniaxial strain. All findings align with a Rashba model in which TRS-protected transport occurs along quasi-1D ferroelastic domain walls, which possess a Dirac band topology and a giant Rashba spin-orbit coupling, two orders stronger than the 2D interface. Our results deepen the understanding of SrTiO3-based electron systems, unveiling an appealing new platform for quantum engineering.

Understanding environmental effects on crystalline defects for quantum technology

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M4QN II, June 25, 2025, 14:15 - 16:05

Point defects in crystalline semiconductors are leading systems upon which many quantum technologies can be built, from quantum computing to sensing. However, fabrication processes such as ion implantation will necessarily lead to the presence of other defects, and experimental work has suggested that these can have a significant influence on properties. Here, we thoroughly examine from first principles how interstitial defects can influence the properties of two colour centres in diamond - the N-V and Sn-V centres. We explore the possible configurations of the system with machine learning potentials, before considering excited state properties of the lowest energy configurations, using linear-scaling time-dependent density functional theory, and the coupling of vibrations to these excitations. We find that the influence of interstitials can have a significant effect on observable quantities, and that this can explain experimental data. This suggests such effects must be carefully controlled when fabricating these systems for practical applications.

Towards a micromechanical qubit based on quantized oscillations in superfluid helium

Dr Priya Sharma¹, Jens Koch², Eran Ginossar¹ ¹University of Surrey, United Kingdom, ²Northwestern University, USA

2D and Topological Physics, June 27, 2025, 10:30 - 12:00

Superconducting circuits can exhibit quantized energy levels and long coherence times. Harnessing the anharmonicity offered by Josephson junctions, such circuits have been successfully employed as qubits, quantum limited amplifiers and sensors. Superfluidity is in many respects the charge-neutral analogue of superconductivity with dissipationless mass flow. Josephson tunneling has been demonstrated in superfluid helium. In this work, we propose a quantum device, consisting of a superfluid weak link and a mechanical element. The superfluid motion in this device is quantized. The resulting discrete energy levels are resolvable at millikelvin temperatures essential to maintaining the superfluid state. Appropriate device engineering can yield the necessary nonlinearity to realize qubit functionality. Hence, this device can potentially operate as a charge-neutral, superfluid quantum bit with micron-sized dimensions and millisecond scale coherence time. We show that this quantum regime is within reach for a range of device designs. This regime profers a novel superfluid device to expand the search for quantum ground states in macroscopic mechanical systems.

Fast Ultraviolet-C Photonics: Sensing Laser Pulses on Femtosecond Timescales

B. T. B. T. Dewes¹, T. Klee², N. D. Cottam¹, J.J. Broughton², M. Shiffa¹, T. S. Cheng¹, S. V. Novikov¹, O. Makarovskiy¹, J.W.G. Tisch², <u>Amalia Patane¹</u> ¹University of Nottingham, United Kingdom, ²Blackett Laboratory, Imperial College London, United Kingdom

2D Materials and Toplogical Devices, June 24, 2025, 14:15 - 16:05

Photonic devices operating in the ultraviolet UV-C range (100-280 nm) have diverse applications from super-resolution microscopy to optical communications, and their advances promise to unlock opportunities in science and technology. However, detecting ultrafast UV-C signals remains a major challenge. This work combines for the first time the generation of femtosecond (fs) UV-C laser pulses with their fast detection by two-dimensional (2D) semiconductors (2DSEM).

We exploit phase-matched second-order processes in nonlinear optical crystals for generation of UV-C laser light. We present two approaches to detection of the fs UV-C laser pulses. These include the 2DSEM GaSe with strong absorption resonances in the UV-C and its oxide [1-3]. Unexpectedly, these 2D sensors exhibit a linear to super-linear photocurrent response to pulse energy, a highly desirable property, laying the foundation for UV-C photonics operating on fs timescales [3]. To date, this capability has not been demonstrated with traditional semiconductors.

The generation and detection of UV-C laser pulses can impact many applications, such as freespace communication between autonomous systems and robotics. We show that a message can be coded by the UV-C laser source-transmitter and decoded by the sensor-receiver [3]. With the efficient generation of UV-C laser light by nonlinear optical processes, we envisage a versatile use of the proposed source-sensor system for different technologies.

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Achieving topological superconductivity with artificial Kitaev chains.

Dr Greg Mazur¹

¹Department Of Materials, University Of Oxford, United Kingdom

Unconventional Superconductivity II, June 26, 2025, 14:15 - 16:05

Majorana zero-modes (MZMs) are predicted to be hosted at the edges of one-dimensional pwave superconductors. MZMs can be characterized as spinless, chargeless and zeroenergy excitations. Interest in MZMs has been driven by their potential applications in quantum computing, where quantum

information can be protected from decoherence. Various platforms where MZMs might be hosted have been proposed, including topological insulators, semiconducting nanowires with strong spin-orbit interaction, iron-based superconductors, and fractional quantum Hall systems. A bottom-up approach has recently been introduced, wherein quantum dots in semiconductors with strong spin-orbit coupling have been coupled through superconductors to create a unit cell of the Kitaev chain[1,2]. Pairs of fine-tuned MZMs can be generated even in such minimal units, through which their properties can be studied [3].

In this talk I will present an experimental approach to the engineering of basic Kitaev chain components in a semiconductor/superconductor hybrid based on InSb nanowires with aluminum half-shells. I will discuss results on chain scaling [4] along with future experiments through which quantum information applications might be implemented using this platform.

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Imaging Odd-Parity Quasiparticle Interference in the Superconductive Surface State of UTe2

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Unconventional Superconductivity, June 26, 2025, 10:30 - 12:50

Although no known material definitely exhibits intrinsic topological superconductivity, where a spin-triplet electron pairing potential $\Delta(k)$ has odd-parity. $\Delta(-k)=-\Delta(k)$. UTe2 is now the leading candidate. Ideally, the parity of $\Delta(k)$ might be established by using Bogoliubov quasiparticle interference (QPI) imaging, a recognized technique for $\Delta(k)$ determination in complex superconductors. However, odd-parity superconductors should support a topological, quasiparticle surface band (QSB) on crystal termination surfaces only for energies within the superconductive energy gap $|E| \leq \Delta$. The QPI should then be dominated by the QSB electronic structure k(E) and only reveal bulk $\Delta(k)$ characteristics excursively. Here, by using a superconducting scan-tip for UTe2 QPI studies, we discover and visualize the in-gap guasiparticle interference patterns of its OSB. Specifically, at the UTe2 (0-11) cleave surface a unique band of Bogoliubov quasiparticles appears only in the superconducting state T<T_c; QPI visualization then yields a characteristic sextet q i:i=1-6 of interference wavevectors from which we establish QSB dispersions k(E), and their existence only for energies $|E| \le \Delta_{max}$ within the range of Fermi momenta projected onto the (0-11) crystal surface. Quantitative evaluation of this sextet q i then demonstrates how the OSB is projected from the subtending bulk Fermi surface. Finally, a novel theoretical framework has been developed to predict the QPI signatures of a topological QSB at this (0-11) surface. Its predictions are demonstrably consistent with the experimental results if the bulk $\Delta(k)$ exhibits time-reversal conserving, oddparity, a-axis nodal, B3u symmetry. Ultimately, these new techniques outline a novel spectroscopic approach to identification of intrinsic topological superconductors and their superconductive topological surface states.

Variational Autoencoder Representation Learning for Break-Junction Data Analysis

Dr Sam Harley1

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Computational Physics, June 25, 2025, 10:30 - 12:50

Break-junction experiments are a powerful tool for the characterisation of single-molecule junctions, and can reveal a wealth of information about the junction throughout the process of formation, stretching, and breaking. However, sophisticated data analysis is required to fully utilize the large datasets produced.

The formation of molecular junctions in break-junction experiments is stochastic, and a complete dataset consists of measurements of thousands of individual junctions. Traditionally, histogram-based analysis is used to extract average properties from the entire dataset; this method is insensitive to more subtle structure within the dataset, resulting in loss of information. For example, a large dataset may contain information about changes in electrical conductance, breaking length and formation likelihood for different junction configurations, which is inaccessible by simple histogram-based analysis approaches.

Recently, there has been increasing interest in applying machine learning to extract additional information from break-junction datasets. Often, clustering algorithms are used to identify subsets of similar junctions, providing insight beyond average properties. Unfortunately, applying clustering algorithms directly yields poor performance due to the high dimensionality of break-junction data. Feature extraction techniques, which map the data to a lower dimensional representation, can be used to address this issue.

In this work, an exploration of variational autoencoder networks for feature extraction of breakjunction data has been conducted, using procedurally generated and experimental datasets to identify strategies to improve upon autoencoder-based methods previously used in breakjunction contexts, towards enhanced clustering accuracy and interpretability.

Estimating Entropy from Coarse-grained Single-molecule Statistics in Langevin Systems

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Non-equilibrium, June 26, 2025, 10:30 - 12:50

Important biological processes at the subcellular level often take place out of equilibrium. Establishing if, when, where and how much these processes dissipate energy provides key insights but is made difficult by environmental thermal fluctuations. Furthermore, the corresponding entropy production can only be measured with complete knowledge of the stochastic trajectories of all the degrees of freedom, which are not typically experimentally accessible. In this work, we develop a technique to obtain a lower bound for the entropy production of generic Langevin systems requiring only the initial and final positions of molecules in a fixed time window, which is experimentally accessible with single-particle tracking.

We study the bound analytically on solvable non-equilibrium steady states of overdamped Langevin systems, allowing us to ascertain under what conditions we capture most of the dissipation of the process, and how to spatially profile entropy density. We validate the method experimentally on the Talin-R3 protein driven out of equilibrium by magnetic tweezers. Our measurement estimates the magnitude of dissipation of protein folding dynamics under physiologically relevant forces, recovering that most of the dissipation occurs during folding and unfolding events. Furthermore, the results offer insights on the biomechanical properties of the protein, such as asymmetries in the free-energy landscape.

This method promises wide applicability to Langevin systems that are ubiquitous in the mesoscopic world, and is valid under steady-state and transient conditions. It is model-free, requiring no specific knowledge of the acting forces or extent of the fluctuations and is data-efficient. A manuscript is in preparation.

Strain-tuning of electronic structure of a tetragonal iron-chalcogenide superconductor

Professor Amalia Coldea¹

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Unconventional Superconductivity II, June 26, 2025, 14:15 - 16:05

The electronic nematic phases of iron chalcogenide manifest themselves in significant orbitallydependent electronic anisotropies and have profound influence on the emerging superconducting state [1,2,3]. In this angle-resolved photoemission study we applied uniaxial strain in a tetragonal iron-chalcogenide superconductor and track the evolution of the induced electronic anisotropies. We identify orbitally-dependent band shifts and changes in the spectral weight function under applied strain [4]. Interestingly, we detect that these changes are similar to those found inside the nematic electronic phase of iron-chalcogenides.

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Triangular antiferromagnetism under uniaxial stress: a study of PdCrO2.

Prof. Clifford Hicks¹

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Magnetism, June 24, 2025, 10:30 - 12:50

PdCrO2 is a triangular Heisenberg antiferromagnet, that shows 120 degree magnetic order below 39 K. The nearest-neighbour magnetic interaction varies strongly with bond length, which allows large deformation of the magnetic order to be induced with modest applied uniaxial stress. Uniaxial stress drives the magnetic order in the Cr layers towards a nesting condition of the Fermi surface in the Pd layers, and, eventually, a first-order transition in which the magnetic order locks in to the nesting condition. In this talk, we will show how the deformation of the magnetic order, including this transition, affects the elastic properties of PdCrO2.

Optimal parallelisation strategies for flat histogram Monte Carlo sampling

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Statistical and Nonlinear, June 25, 2025, 10:30 - 12:50

Flat histogram methods such as Wang Landau sampling [1] provide a means for high throughput calculation of phase diagrams for atomistic/lattice model systems. Many parallelisation schemes have been proposed to accelerate sampling simulations with varying degrees of complexity [2]. In this study, these different schemes are benchmarked—both in isolation and in combination—to establish best practice. The schemes studied include energy domain decomposition with both static domains and a dynamic domain sizing which we propose. We also assess the benefit of replica exchange and including multiple random walkers per domain to determine which factor has the largest impact on parallel efficiency. The influence of flatness criteria and domain overlap will also be discussed. As illustrative test cases, we implement and apply the aforementioned strategies to a lattice-based model describing the internal energies of the the AlTiVNb and AlTiCrMo refractory high-entropy superalloys, both of which are understood to crystallographically order into a B2 (CsCl) structure with decreasing temperature [3].

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Competing aggregation and iso-density equilibrium lead to band patterns in density gradients

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Statistical and Nonlinear, June 25, 2025, 10:30 - 12:50

Centrifugation of erythrocytes (aka Red Blood Cells, RBCs) in self-forming percoll gradient is a protocol often used as a way to sort RBCs by age. However, a pattern formation of discrete bands is systematically observed along the continuous density gradient. Although early studies mentioned that aggregation between cells might modify their spatial distribution, it is debated whether a population with continuous density distribution can form discrete bands. Here, we develop a continuous equation, considering the aggregation of cells with a continuous density distribution, which describes the macroscopic evolution of RBCs concentration in a density gradient. Using numerical resolutions, we demonstrate that the competition between isodensity distribution and aggregation is sufficient to create band patterns. Our model reproduces gualitatively the temporal evolution observed in the conventional experimental protocol, but also predicts several types of bifurcation-like behaviors for the steady-state patterns in constant gradients, when the volume fraction and aggregation energy of the cells are varied. We developed an experimental protocol where a constant density gradient is formed and where the results of the model match the observed patterns. The competition between aggregation and iso-density distribution is therefore a novel physical mechanism leading to a new and rich pattern formation system.

High-temperature superconductivity in thin-film metal hydrides at megabar pressures

<u>Dr Sam Cross</u>¹, Owen Moulding^{1,2}, Israel Osmond^{1,3}, Annabelle Brooks¹, William Thomas¹, Xiaojiao Liu⁴, Annette Kleppe⁴, Nico Giordano⁵, Timofey Fedotenko⁵, Hanns-Peter Liermann⁵, Bjorn Wehinger⁶, Mohamed Mezouar⁶, Alix McCollam^{7,8}, Toni Helm^{9,10}, Oliver Lord¹¹, Sven Friedemann¹, Jonathan Buhot¹

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Superconductivity I (IOP SC Group), June 24, 2025, 10:30 - 12:50

At present, compressed metal hydrides exhibit the highest superconducting critical temperatures amongst all known materials [1-3]. The current record is held by lanthanum decahydride, LaH10, with Tc ~ 250 K at pressures close to 200 GPa [2,3]. The synthesis and characterisation of such compounds presents a significant experimental challenge owing to the extreme pressures required, and the difficulties in synthesising single-phase superconducting samples. In this talk, I will present an overview of the experimental studies of hydride superconductors conducted at the University of Bristol, including confirmations of high-Tc superconductivity in H3S [4], YH4, LaH4, LaH10, and La4H23 [5]. I will outline our novel thinfilm techniques for the preparation of electrodes and high-Tc hydride samples in diamond anvil cells [4-6]. I will focus on our recent discovery of high-Tc superconductivity in La4H23 [5] with Tc ~ 90 K below 100 GPa – the highest Tc amongst known type-I binary clathrate hydrides to date. The novel structure is characterised using synchrotron powder XRD, and superconductivity evidenced using electrical resistivity measurements in magnetic field, allowing mapping of the magnetic phase boundary Hc2(T). I will also discuss the remaining challenges for hydride synthesis at such extreme pressures.

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- [6] Phys. Rev. B 102, 104508 (2020)

Molecular Insights into Irregular Growth of Salt Crystals: The Role of Charge and Water Structure

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Materials for Energy and Chemical physics and Self-Assembly, June 27, 2025, 10:30 - 12:00

Salt crystal growth from supersaturated solutions is a fundamental process in both the environment and engineering systems, playing a critical role in phenomena such as soil salinization and salt crust formation. Despite its importance, the molecular-scale mechanisms that govern salt crystal growth remain incompletely understood. Recent work has highlighted how interfacial phenomena-particularly water structuring, local roughness, and surface charge-can decisively affect water transport in porous salt crusts. Here, we use molecular dynamics simulations to analyze how these factors drive the precipitation of three common salts (NaCl, KCl, and Na₂SO₄) on pre-existing crystal surfaces under controlled supersaturation. We find that although the net crystal growth for all three salts proceeds linearly over microsecond timescales (with similar rates), their growth morphologies differ strikingly. Specifically, in NaCl and Na₂SO₄, preferential cation adsorption can lead to multilayered, rough growth: Na⁺ ions preferentially adsorb to the crystal surface, resulting in charge build-up, which subsequently triggers the growth of the next layer much before the underlying layer is complete. This results in the growth of irregular surfaces that deviate from classic layer-by-layer growth. We identify the origin of this anomalous crystal growth by examining the adsorption energy of ions at specific topological defects, such as steps and kinks on the crystal surface. Local variations in electrostatic potential and water structuring generate surface sites that selectively favor the adsorption of ions or the retention of water molecules. These findings offer detailed insights into the molecular mechanisms of salt crystal growth and have implications for understanding salt precipitation.

Simulating 23Na NMR of sodium-ion-modified ZIF-62 glass

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Materials for Energy and Chemical physics and Self-Assembly, June 27, 2025, 10:30 - 12:00

ZIF-62 is a mixed-linker metal-organic framework known for its exceptionally high glass-forming ability. Taking inspiration from silicate-based glass techniques, modifying glassy ZIF-62 with Na+ substantially lowers its glass transition temperature, which promises to improve its overall processability. Here, we simulated 23Na NMR via DFT GIPAW on Na-ZIF-62 to determine the mechanisms responsible for its decreased transition temperature. Over 300 Na+ environments were generated and classified according to their match with experimental NMR spectra. We found Na+ substitution in ZIF-62 distorts the framework and reduces connectivity, leading to 4- or 3-coordinated Na+. This contrasts the 6- or 5- coordinated Na+ in Na-modified silicate glasses. The unique structural role of Na+ in Na-modified ZIFs highlights the potential to adapt glass modification principles to MOF-based systems, achieving new structural and functional outcomes.

Physics and materials science of elemental uranium thin films and alloys

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Strongly Correlated Materials, June 24, 2025, 14:15 - 16:05

Thin films offer a myriad of ways of controlling and tuning states of matter. We can apply epitaxial strain, vary the dimensionality, and combine different order parameters together using proximity effects to name but a few of the possibilities [1]. In this talk I will briefly describe two case studies of engineering structural and electronic states with thin films. First, I will show an intriguing study of a topotactic phase transition in elemental U between an epitaxy-induced metastable hexagonal-close-packed phase, and the bulk ground-state, the orthorhombic structure [2]. Second, I will introduce using alloys of U and Nb to study the use of spin-orbit physics to generate novel superconducting order parameters in polycrystalline films [3].

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Figure 1: Specular scans of a 1400 Å hexagonal-close-packed U film grown onto a polycrystalline Cu{111} surface over the first seven days following growth. Arrows indicate the direction of growth/decay of the Bragg peaks. The dashed line represents the position of the bulk U orthorhombic (002) reflection. Taken from Ref. [2].

Breaking symmetry to save symmetry with rejection-free Monte Carlo

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Statistical and Nonlinear, June 25, 2025, 10:30 - 12:50

The famous Metropolis algorithm [1] was the original Monte Carlo sampling algorithm. It has enjoyed huge success across the physical and statistical sciences, but typically exhibits slow mixing when faced with broken symmetry in statistical physics — as well as very strong autocorrelations at phase transitions. This is often due to a high rate of rejected moves, but more recent developments [2, 3] have led to a new class of rejection-free Monte Carlo algorithm. Event-chain Monte Carlo augments the state space with auxiliary momenta, which leads to ballistic-style dynamics that drive the system through the original state space and without rejection. Moreover, breaking symmetry on momentum space can recover symmetry on the original state space [4] — a concept that also accelerated mixing in the seminal work that solved the 2D melting transition [5].

We start this talk with a brief introduction to event-chain Monte Carlo. We then take a fresh look at broken symmetry by comparing Metropolis and event-chain simulations of the 2DXY model at low temperature, before reflecting on how the event-chain simulations achieved symmetry on the original state space by breaking symmetry on momentum space [4]. We finish by looking to the future in terms of alleviating strong autocorrelations at the phase transition itself. Moreover, analogous strong autocorrelations develop in the continuum-time limit of the Feynman path-integral approach to computational quantum mechanics. We present some very recent event-chain work that alleviates these issues — in particular when relaxing the system if far from equilibrium.

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Identification of topological superconductivity in antiferromagnetic heavy-fermion metal YbRh2Si2

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Unconventional Superconductivity, June 26, 2025, 10:30 - 12:50

We report a study of superconductivity in a tetragonal heavy fermion metal YbRh2Si2 through SQUID-based measurements of complex electrical impedance down to ultra-low temperatures [1]. The superconductivity stabilises below 10 mK on the background of rich magnetism, featuring an electronic antiferromagnetic (AFM) phase of unknown magnetic structure with onset at TN = 70 mK and an electro-nuclear spin-density wave (SDW) below TA = 1.5 mK [2].

The presence of multiple transport signatures in each single crystal sample and strong sampleto-sample variations reveal that the superconductivity is heterogeneous: different regions of the samples exhibit superconducting states distinctly suppressed by magnetic field, both Pauli limited and exceeding this Pauli-limiting field by an order of magnitude. This provides strong evidence for odd-parity spin-triplet pairing in YbRh2Si2. We identify the state with in-plane Pauli limit with a helical order parameter, corresponding to the planar phase of superfluid 3He, with non-trivial momentum-space topology [3].

A striking observation is the boost of the helical state and simultaneous suppression of other superconducting states at the onset of electro-nuclear SDW at TA. We attribute this selective boost to the formation of a spin-triplet pair density wave (PDW) that attractively couples the magnetic and superconducting order parameters.

The low transition temperatures in YbRh2Si2 confer advantages through modest energy scales: the magnetism and superconductivity are effectively tuneable by modest magnetic field, uniaxial strain and Yb isotopic substitution. This flexibility makes YbRh2Si2 a promising material for topological superconducting technology.

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Tunable Ultra-Strong Magnon-Magnon Coupling Approaching the Deep-Strong Regime in a van der Waals Antiferromagnet

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Spin-Orbit, June 24, 2025, 14:15 - 16:05

Antiferromagnetic (AFM) magnons in van der Waals (vdW) materials offer substantial potential for applications in magnonics and spintronics. In this study, we demonstrate ultra-strong magnon-magnon coupling in the GHz regime within a vdW AFM, achieving a maximum coupling rate of 0.91. Our investigation shows the tunability of coupling strength through temperature-dependent magnetic anisotropies.

Additionally, analytical calculations show the possibility to reach the deep-strong coupling regime by engineering the magnetic anisotropy. These findings highlight the potential of vdW AFMs as a model case to study magnetisation dynamics in low-symmetry magnetic materials.

Spintronic Kapitza pendulum: dynamical stability by spin transfer

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Spin-Orbit, June 24, 2025, 14:15 - 16:05

Spin transfer torques (STTs) control magnetisation by electric currents, enabling a range of spintronic applications [1-2]. STTs are in general employed in switching the magnetisation from one local energy minima to the other or in entering auto-oscillation but so far only these two have been studied as non-linear dynamics driven by STTs.

Inspired by the Kapitza pendulum [3] where a high potential energy state can be stabilised by dynamical injection of mechanical force (Fig.a), here we study the spintronic analogue of such a state achieved by nonequilibrium excitation of STTs. To achieve the same potential landscape with only one global potential minimum (Fig. c), and to maximise the efficiency of current-driven STTs, we made a dedicated CoFeB thin film layer with a characteristic property of the nearly-isotropic magnet. We use STTs generated by spin-Hall effect in the adjacent W layer to de-stabilise the energy minimum state achieved by an external field and observed the experimental signature of stabilising the state at the energy maxima, i.e. the moment pointing at the direction opposite to the external field, when the STT drive is strong enough to compenstate the material damping. One such observation is the sign reversal of ferromagnetic resonance voltage amplitude when increasing the STT drive as shown in Fig. d. Here, for a small current of 4 mA, the magnetisation precession takes place around the external field. At a higher current of 6 mA, the potential maxima condition is achieved, the moment presesses around the direction opposite to field, resulting in the peak sign reversal. We will discuss more technical details of these measurements, quantitative analysis and results by stochastic Landau-Lifshitz-Gilbert equation.

The discovery of a nano-scale rigid pendulum with dynamical stabilisation and controllable stochasticity is an ideal platform for studying dynamical systems with promising functionalities for probabilistic computing applications [4] and anti-magnonics [5].

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a&**b**: Schematics of mechanical and spintronic Kapitza pendulums. **c**: Schematic of destabilization of the state from the energy minima to stabilization of the energy maxima. **d**: FMR voltages for different STT drives by dc currents.

Non-Markovian Quantum Mpemba Effect

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Non-equilibrium, June 26, 2025, 10:30 - 12:50

Since its rediscovery in the twentieth century, the Mpemba effect, where a far-from-equilibrium state may relax faster than a state closer to equilibrium, has been extensively studied in classical systems and has recently received attention in quantum systems. Many theories explaining this counter-intuitive behavior in classical systems rely on memory effects. However, in guantum systems, the relation between the Mpemba effect and memory has remained unexplored. In this work, we consider general non-Markovian open quantum systems and reveal new classes of quantum Mpemba effects, with no analog in Markovian quantum dynamics. Generically, open quantum dynamics possess a finite memory time and a unique steady state. Due to non-Markovian dynamics, even if the system is initialized in the steady state it can take a long time to relax back. We find other initial states that reach the steady state much faster. Most notably, we demonstrate that there can be an initial state in which the system reaches the steady state within the finite memory time itself, giving the fastest possible relaxation to stationarity. We verify the effect for quantum dot systems coupled to electronic reservoirs in equilibrium and non-equilibrium setups at weak, intermediate and strong coupling. Our work provides new insights into the rich physics underlying accelerated relaxation in quantum systems.

From continuum excitations to sharp magnons via transverse magnetic field in the spin-1/2 Ising-like triangular lattice antiferromagnet Na2BaCo(PO4)2

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Magnetism, June 24, 2025, 10:30 - 12:50

The lsing-like spin-1/2 triangular lattice antiferromagnet is one of the theoretically most studied paradigms of a frustrated quantum spin model. We report high-resolution inelastic neutron scattering measurements that observe the evolution of the spectrum as a function of transverse magnetic field in a disorder-free material realization of this model. We reveal how the excitation continuum in zero field transforms via an intermediate-field phase with broadened magnons into a spectrum of sharp magnons in the polarized phase at high field. We propose that the origin of the dominant continuum of excitations in zero field is related to the existence of a mean-field degenerate manifold of ground states and compare the experimental data with the expected spectrum of excitations in this case.

Ultraclean contacts for two-dimensional spintronic and ferroelectric memory devices

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2D Materials and Toplogical Devices, June 24, 2025, 14:15 - 16:05

Ferroic devices based on two-dimensional (2D) materials offer transformative solutions for high-density, non-volatile memory at advanced technology nodes. However, realising their full potential requires overcoming challenges related to device yield, reliability, and performance.1 One critical challenge is to achieve clean metal contacts for 2D spintronic and ferroelectric memory devices. Here, we demonstrate how clean ferromagnetic van der Waals (vdW) contacts of indium and cobalt can enable spin-injection in graphene at room temperature, resulting in magnetoresistance over 15 times higher than defective contacts with pure cobalt. By leveraging spin tunneling through the vdW gap, we eliminate the unreliable step of depositing ultrathin dielectric tunnel barriers on 2D surfaces, improving device yield. Non-local spin transport is observed at room temperature. We also show that clean contacts improve the electroresistance of ferroelectric diodes (FeDs) based on vdW heterostructures of CuInP2S6 (CIPS. <10 nm thick) and graphene, achieving ON/OFF ratios around 106, rectification ratios above 2500, low read/write voltages of 0.5/2V and a maximum output current density of 100 A/cm2. The improved performance can be attributed to due to the absence of interface defects which allows effective modulation of the average barrier height upon polarisation switching. In addition, the stabilisation of intermediate net polarisation states in CIPS leads to multi-bit data retention at room temperature. Combined with its two-terminal self-selecting design, FeDs based on vdW heterostructures provide a viable approach for high-density compute-in-memory applications.

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Critical spin fluctuations and strange metal behaviour in La2-xSrxCuO4

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Strongly Correlated Electron Systems, June 26, 2025, 14:15 - 16:05

High Tc cuprate superconductors are a family of oxides with numerous competing phases such as anti-ferromagnetism, spin or charge density wave order and high-temperature superconductivity which can be tuned via doping [1]. At higher dopings away from any ordered state, cuprates exhibit strange or anomalous normal state properties including resistivity $\rho \propto T$ down to the lowest accessible temperatures [2]. It has been held that only a strongly temperature-dependent 'Planckian' scattering rate, $\hbar T-1 = akBT$ (a ~ 1), in the inelastic sector can necessarily explain these observations.

Motivated by this, we have studied the evolution of low-energy ($\hbar \omega \sim kBT$) spin fluctuations in La2-xSrxCuO4 x=0.22 and x=0.19 over the temperature range of strange metallic behaviour. p*, the doping at which the pseudogap closes, is held to be close to p = x = 0.19. In the higher doped sample, we have found clear evidence of dynamical critical scaling, including energy-temperature (ω /T) scaling, in the normal state. This is associated with proximity to a quantum critical point. In other words, the temperature dependence of the spin susceptibility χ (Q, ω) is controlled by a thermal correlation length $\xi T \sim T-1/z$ down to at least Tc = 26K (measurements were not taken in the superconducting state). For x=0.19, the presence of a fixed ~8meV energy scale complicates matters however the temperature dependence of the low-energy slope, $\chi''(Q, \omega)/\omega$, is nonetheless well-described by the same power law as at x=0.22. These results suggest a strong link between critical spin fluctuations and the aforementioned regime of unconventional transport.

Recent numerical calculations on a Yukawa-Sachdev-Kitaev-Ye (YSYK) model have also come to the same conclusions. Here, dynamical critical scaling in $\chi''(Q, \omega)$ goes hand in hand with T-linear resistivity for $\lambda > \lambda c$, λ is a tuning parameter equivalent to doping. This is owing to an extended quantum Griffiths phase induced by the disorder.

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Emergent exchange-driven giant magnetoelastic coupling in a correlated itinerant ferromagnet

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Strongly Correlated Electron Systems, June 26, 2025, 14:15 - 16:05

The phenomenology and radical changes seen in the properties of materials which exhibit strong electron correlations has captivated condensed matter research over the past decades. Correlations lead to novel ground states, including magnetic order, nematicity and unconventional superconductivity, yet the driving mechanism behind these is still unresolved, and they often exhibit surprising sensitivity to modest stimuli. Here, we demonstrate how in a correlated material, Sr4Ru3010, magnetic interactions couple to lattice degrees of freedom resulting in a giant magnetoelastic coupling. We establish control of the magnetism in the surface layer and use this control to probe the impact of the magnetism on its electronic and structural properties. By using scanning tunneling microscopy (STM), we reveal subtle changes in the electronic structure dependent on ferromagnetic or antiferromagnetic alignment between the surface and subsurface layers. We determine the consequences of the exchange force on the relaxation of the surface layer, exhibiting a giant magnetostriction. Our results provide a direct measurement of the impact of exchange interactions and correlations on structural details in a quantum material, reveal how electronic correlations result in strong electron-lattice coupling and establish Sr4Ru3010 as a model system to study magnetism in 2D.

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Carolina A. Marques, Luke C. Rhodes, Weronika Osmolska, Harry Lane, Izidor Benedičič, Masahiro Naritsuka, Siri A. Berge, Rosalba Fittipaldi, Mariateresa Lettieri, Antonio Vecchione, and Peter Wahl, Emergent exchange-driven giant magnetoelastic coupling in a correlated itinerant ferromagnet, arxiv/2505.09611, to appear in Nature Physics.

Magnetised Haldane Chain

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Strongly Correlated Materials, June 24, 2025, 14:15 - 16:05

We report on the magnetic properties of the S=1 Haldane chain material Nil2(C7H9N)4 with particular focus on its magnetized state. Magnetisation measurements at the lowest measured temperature of 0.36 K indicate the realisation of a Tomonaga-Luttinger (TLL) ground state. However, signatures of TLL behaviour vanish already at 1.8 K, despite he exchange interaction energy being on the order of 17.5 K. NMR relaxation rate measurements in the gapless, magnetised regime exhibits a power-law temperature dependence. However, the extracted exponent of 1.2 lies well outside the expected TLL range between -2/3 and 1/2, pointing to the emergence of a previously unrecognised low- to intermediate-temperature regime, distinct from both the TLL and high temperature paramagnetic limits.

Poster Presentations

DFT+U Study of Magnetic Configurations and 5f Electron Behaviour in UAu_2

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Poster Session, Exhibition, Drinks Reception and Buffet, June 24, 2025, 17:30 - 19:30

UAu₂ is a uranium-based compound where a frustrated stacked triangular lattice of uranium atoms leads to rich and unusual magnetic behaviour, including an incommensurately modulated antiferromagnetic state that exhibits non-Fermi liquid characteristics [1,2], a fieldinduced transition to a ferrimagnetic state [2], as well as the emergence of multicomponent odd-parity superconductivity at high pressure [3]. In this project, the DFT+U method was used to explore how different magnetic configurations (non-magnetic, ferromagnetic and ferrimagnetic) affect the structure and electronic properties of UAu₂. Structural optimizations and total energy comparisons across a range of Hubbard U values were carried out to assess the relative stability of these configurations, indicating that the ferrimagnetic state is likely the most stable. We also examined the band structure and density of states, where the uranium 5f electrons show strong sensitivity to U, becoming more localized and spin-polarized with increasing values. These changes significantly impact hybridization with the gold 5d states. In addition, the Fermi surface of the ferrimagnetic state is compared to quantum oscillations observed in recent measurements. While this work focuses on UAu₂, it also lays the foundation for exploring other strongly correlated systems. By combining theoretical predictions with experimental observations, this study aims to deepen our understanding of the complex behaviour found in uranium-based heavy fermion materials.

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Tunability of spin texture in conformally-coated 3D nanostructured magnetic metamaterials

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Poster Session, Exhibition, Drinks Reception and Buffet, June 24, 2025, 17:30 - 19:30

The transition from planar to 3D magnetic nanostructures offers significant potential for ultrahigh-density data storage, neuromorphic computing and the exploration of exotic physical phenomena [1]. Line-of-sight deposition of magnetic material onto 3D polymer nanoscaffolds, fabricated via two-photon lithography (TPL), introduces a shadowing effect which limits the number of magnetic layers available, whilst techniques involving the direct fabrication of 3D magnetic nanostructures struggle to fabricate the necessary complex, high-purity structures over a large area. A recently demonstrated [2] solution is to use TPL to realise a polymer nanostructure and then coat with a ferromagnetic material such as Ni via atomic layer deposition, allowing the creation of complex arbitrary 3D magnetic nanostructures. Here, we use this method to fabricate networks of ferromagnetic nanotubes arranged in a woodpile geometry with a varying number of Ni tubes stacked in the out-of-plane direction (z). Woodpiles with a lower number of stacked nanotubes favour a chiral configuration whereby the magnetisation wraps around the cross-section of the top-most tube. As further nanotubes are added in z, a transition occurs into a more uniform configuration, whereby the magnetisation predominantly lays along the tube long-axis. The rate at which this transition occurs can be controlled via the lattice period, where a reduced period creates a sharper transition. This work paves the way to tuneable magnetic metamaterials with desired static and dynamic properties.

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Hall Array Magnetometry of Ferromagnetic Iron-Pnictide Superconductor EuFe2(As0.79P0.21)

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Poster Session, Exhibition, Drinks Reception and Buffet, June 24, 2025, 17:30 - 19:30

Ferromagnetic superconductors are a rare class of materials displaying two antagonistic phenomena; magnetic ordering usually suppresses superconductivity by the breaking of spinsinglet Cooper pairs by the strong ferromagnetic exchange interaction. In EuFe2(As1-xPx) ferromagnetism and superconductivity coexist over a large temperature range. The maximum T c = 25 K is at x = 0.21, and uniaxial ferromagnetic ordering sets in below T FM = 19 K. resulting in an ideal system to study the effect of ferromagnetic ordering on superconductivity. Previous studies have used bulk magnetometry, magnetic relaxation and MFM measurements to demonstrate that the magnetic irreversibility is strongly dependent upon the presence of both ferromagnetic and superconducting orders. In the current work, we have used Hall array magnetometry to systematically study the spatially resolved magnetic behaviour of single crystal EuFe2(As0.79P0.21) in several characteristic temperature regimes. In a small temperature window below T FM, in the absence of an applied field, ferromagnetic domains manifest in the form of a striped domain structure with alternating moment directions. known as the domain Meissner state. At lower temperatures, spontaneous vortex-antivortex pairs nucleate in a first order phase transition to the domain vortex state characterised by substantially wider domains.

We will report systematic investigations of the magnetic irreversibility of our samples. We explore how the shape of hysteresis loops changes qualitatively in different characteristic regimes, becoming more dominated by ferromagnetism at the lowest temperatures.

Micromagnetic modelling of Ni nanotubes with circular and elliptical cross-section

<u>Miss Satya Lanka</u>¹, Joseph Askey¹, Sam Ladak¹ ¹Cardiff University, United Kingdom

Poster Session, Exhibition, Drinks Reception and Buffet, June 24, 2025, 17:30 - 19:30

Cylindrical ferromagnetic nanotubes are promising nanostructures for applications in spintronics [1] and data storage [2] due to ultrafast domain wall motion [3]. Magnetisation textures and domain walls in ideal cylindrical nanotube systems have been studied extensively in nanomagnetism [4], but little work has been done to elucidate the magnetisation textures in elliptical cross-section nanotubes. The advent of novel 3D lithographic and deposition technologies paves the way for realising such systems, making it imperative to characterise the expected textures.

Micromagnetic simulations were used to study nickel nanotubes with circular and elliptical cross-sections, defined by (β , major/minor diameter), varying minor diameters (d) and thicknesses (t). Four magnetic states emerge. Circular nanotubes exhibit uniform magnetisation, parallel to the long axis, at small d and t transitioning to mixed states, where magnetisation is uniform in the central region and canted at the extremities, and then curling states, where magnetisation exhibits azimuthal alignment, as d and t increase. In the experimentally realisable range (β =1, d=200 nm, t=50 nm), a metastable surface vortex (SV) state appears. For elliptical nanotubes (β >1), similar uniform and mixed states arise at small d and t, but for large β , a stable SV state emerges, characterised by coupled vortex pairs on sidewalls. The results indicate that curvature enables precise control of ground state magnetisation textures in experimental nanowire systems.

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Topological Solitons and Monopolar Fields in a 3D Artificial Spin-Ice

Dr Arjen van den Berg¹, Peter Rickhaus², Sam Ladak¹ ¹Cardiff University, United Kingdom, ²Qnami AG, Switzerland

Poster Session, Exhibition, Drinks Reception and Buffet, June 24, 2025, 17:30 - 19:30

Artificial spin-ices are lattices of single-domain magnetic nanowires arranged to allow direct exploration of physics associated with frustration [1] and emergent magnetic monopole-like defects [2], with recent work realising 3D artificial spin ice (3DASI) systems demonstrating magnetic monopole transport [3] and the formation of charge-ordered states [4]. Driven by recent interest in topological states in stray fields of 3D magnetic nanostructures, we employ nitrogen vacancy (NV) magnetometry to explore stray fields of 3DASI in controlled magnetic configurations. Bolstered by micromagnetic simulations, we identify topological structures in the stray field of 3DASIs and explore the highly divergent monopole defect fields and deviation from idealised point sources. These results highlight the utility of NV magnetometry in 3D nanomagnetism, and demonstrate potential in modulating coulombic interactions in 3DASI for controlled monopole dynamics.

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Vortex dynamics in thin film superconductor ratchet structures

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Poster Session, Exhibition, Drinks Reception and Buffet, June 24, 2025, 17:30 - 19:30

Modern superconducting integrated circuits, which are essential for high-frequency digital signal processing, A/D converters, and superconducting qubits, often experience performance degradation due to trapped flux in the form of quantised superconducting vortices. These vortices lead to increased energy dissipation and noise, ultimately reducing the circuit's efficiency. Here we report a novel approach to mitigate these effects by removing vortices from active sites using external AC magnetic fields and/or AC currents, leveraging the Lorentz force to move the vortices. A superconducting film incorporating a sawtooth ratchet design will be introduced to promote unidirectional vortex motion, driving the vortices in one direction while preventing backwards movement. To inform the design of these structures, we have used scanning Hall probe microscopy to make a vortex-resolved imaging study of a 200 nm thin niobium film under varying applied magnetic fields. The recorded vortex patterns reflect the underlying pinning landscape of the film, revealing regions of very strong pinning which remain occupied by vortices as the applied field increases. The experimentally observed pinning landscape will be incorporated into realistic molecular dynamics computational models of vortex motion. Square wave drives are frequently assumed to model the dynamics of vortex ratchet structures. Here we explore the use of more realistic AC drives which result in a significant decrease in the maximum average vortex velocity for the same drive amplitude.

Measuring the Variation in Zero Temperature Magnetic Penetration Depth of Cuprate Superconductors with Pressure

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Poster Session, Exhibition, Drinks Reception and Buffet, June 24, 2025, 17:30 - 19:30

The Magnetic Penetration Depth (MPD) is an important property of all families of Superconductors and can be linked via the London Equations to the Super Fluid Density and Effective Mass of Charge Carriers. The Cuprates are an extensively studied family of high temperature superconductors which exhibit a superconducting dome in Tc when tuned by doping and pressure. The source of, and explanation for, this behaviour in both the overdoped and underdoped regimes has been the source of much debate₁.

In this work, a novel approach for probing the variation of the Zero Temperature MPD with pressure is developed. This technique involves correlating changes in MPD with frequency changes in an oscillator circuit by positioning the high Tc cuprate sample in an inductor coil and coating the samples with a thin layer of a low Tc superconductor (lead)₂. This coating layer of known MPD allows the absolute value of the MPD of the underlying sample to be ascertained. Pressures of up to 3GPa can then be realised by placing the sample and coil inside a piston cell. Here the technique is shown on Y123 samples to show the evolution of MPD as a function of pressure and doping.

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Demonstrating temperature stability of a closed cycle helium-4 cryomagnetic platform

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Poster Session, Exhibition, Drinks Reception and Buffet, June 24, 2025, 17:30 - 19:30

Being able to achieve high accuracy and stability when controlling temperature is important for characterising the electrical properties of materials. For example, when studying the superconducting properties of strongly correlated systems [1]. Electrical transport properties are also commonly studied as a function of magnetic field. For instance, the study of the quantum Hall effect in 2D materials, such as graphene [2]. Therefore, it becomes necessary to use temperature sensors with limited and predictable magnetoresistance [3]. The closed cycle helium-4 cryo-magnetic platform provides a low temperature and high magnetic field environment suitable for characterising material properties as a function of temperature between 1.5 and 300 K, and up to magnetic fields of 14 T. Here, we demonstrate the temperature stability both at zero field, and for fields of up to 12 T. The temperature is recorded over several hours for temperatures between 2 and 10 K with millikelvin stability. We use this system to measure the superconducting transition of a NbTi wire as a function of magnetic field at a series of discrete temperatures, 150 mK apart, and show the extracted critical field value at 0 K, Bc(T=0 K), to be around 17 T.

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Light-Induced Interlayer Raman Forces in 2D Materials

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Poster Session, Exhibition, Drinks Reception and Buffet, June 24, 2025, 17:30 - 19:30

In general, the Raman effect is a three-wave mixing process, being inelastic scattering of a light generation or annihilation of a vibration, which is a phonon in condensed systems. We instead consider the perspective where the phonon is the outgoing response from a second-order light-matter interaction, meaning that we observe a second-order response which generates a force between atoms, called the Raman force. We look at the case where the phonon is rectified, analogous to a DC photocurrent, meaning we observe a change in the equilibrium positions of atoms (displacive motion) on top of oscillatory (impulsive) motion. Here, we analyse the second-order Raman force susceptibility theoretically using a Feynman diagrammatic approach, describing electron-phonon coupling using a force constant model, from which we identify the displacive and impulsive components for responses to both linearly and circularly-polarised light. We elucidate the quantum geometric-dependence of the key components, as well as the additional components which determine the strength and sign of each particular response, and the effect of symmetry. We also obtain numerical results for a bilayer Haldane model, allowing for the response components to be quantified and visualised with respect to a chosen band structure, over a range of incident frequencies of light.

Improving Strain Measurements of Highly Stressed Quantum Materials

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Poster Session, Exhibition, Drinks Reception and Buffet, June 24, 2025, 17:30 - 19:30

Strain tuning offers a simple but powerful method to drive a material's lattice parameters. Nevertheless, adhesives used to mount samples and stress inhomogeneities increase the strain measurement's uncertainty at high stresses. We demonstrate examples of these impacts and improvements to current apparatuses.

Nanofabrication, characterisation and tuning of Nb3Cl8 via photolithography for Ionic Liquid gating:

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Poster Session, Exhibition, Drinks Reception and Buffet, June 24, 2025, 17:30 - 19:30

Nb3Cl8 is a 2D van der Waals material with a breathing Kagome Lattice, thought to be a prototypical Mott-Hubbard insulator at the monolayer [1]. It has been shown experimentally to exhibit a topological flat band structure, tuneable by doping, and exhibits possible signatures of a Quantum Spin Liquid phase [2]. Recent measurements have demonstrated electrostatic manipulation of this state via field-effect gating [3]. Nb3Cl8 is thus a promising material candidate for controlled exploration of these exotic phases.

Through mechanical exfoliation, we show it is possible to make large (<µm) sized samples of a few monolayers thickness from bulk Nb3Cl8 crystals, suitable for ionic liquid gating. This poster overviews fabrication and characterisation of such devices. Flakes are prepared from bulk Nb3Cl8 as well as doped Nb3 TexCl8-x crystals and contacted by photolithographic lift-off. Flake thicknesses are characterised via optical transparency and atomic force microscopy. We also present preliminary X-ray diffraction and Raman characterisation.

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[2] - Sun, Z., Zhou, H., Wang, C., Kumar, S., Geng, D., Yue, S., Han, X., Haraguchi, Y., Shimada, K., Cheng, P., Chen, L., Shi, Y., Wu, K., Meng, S., & Feng, B. (2022). Observation of Topological Flat Bands in the Kagome Semiconductor Nb3Cl8. Nano Letters, 22(11), 4596–4602. https://doi.org/10.1021/acs.nanolett.2c00778

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Probing the nematic quantum criticality of FeSe1-xSx

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Poster Session, Exhibition, Drinks Reception and Buffet, June 24, 2025, 17:30 - 19:30

The compound FeSe1-xSx hosts a nematic transition in the absence of static magnetism that is suppressed from ~ 90 K to 0 K through Sulphur substitution of the Selenium atoms [1]. Quantum critical fluctuations of the nematic order parameter around this putative quantum critical point are thought to provide a source of superconductive pairing [2]. This poster presents recent work to precisely locate the nematic critical point through EDX, WDS and low temperature XRD studies of a set of overdoped FeSe1-xSx bulk samples. These measurements are combined with an ongoing project tracking the A coefficient of low temperature T2 resistivity when approaching the putative critical point from the overdoped regime, thus testing the influence of nematic critical fluctuations on the electronic state [2]. Examples of FeSe1-xSx devices manufactured using FIB techniques are also presented, with a description of how μ m-scale samples with complex geometries can open the door to more advanced and robust transport studies [3].

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100 kHz Repetition Rate Extreme Ultraviolet Beamlines at the Artemis Facility

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Poster Session, Exhibition, Drinks Reception and Buffet, June 24, 2025, 17:30 - 19:30

The Artemis laboratory at the UK's Central Laser Facility (CLF) is a user facility offering access to high average power femtosecond laser systems and HHG sources for a variety of ultrafast extreme ultraviolet (XUV) experiments. The XUV beamlines provide the capability for time-and angle- resolved photoemission spectroscopy (TR-ARPES) on solid samples, and photoelectron spectroscopy (PES) with tunable optical and infrared pump pulses and XUV probe pulses. TR-ARPES with high harmonic probe pulses have enabled studies of electron dynamics in charge-ordered 2D materials. We use a 100 kHz optical parametric chirped pulse amplification system to drive the HHG source. We have also upgraded our TR-ARPES endstation with a new Fermi surface mapping analyser, enabling efficient acquisition of high-quality ARPES spectra of optically pumped excitations close to the Fermi surface level.

We have recently secured funding for a £17M major upgrade of all the CLF's ultrafast facilities. The upgraded Artemis will offer new 100 kHz laser system with a tunable wavelength from 230 nm to 10 microns. A new materials science end-station will offer a momentum microscope and a hemispherical analyser for time- and angle-resolved photoemission and state-of-the-art material preparation and characterisation.

We aim to expand the facility's capabilities with the addition of a new beamline that will generate broadband XUV pulses for time-resolved XUV and soft-X-ray absorption spectroscopy in liquid- and gas-phase samples and perform XUV ptychographic imaging of microscopic samples.

The new facilities will be available to access starting in 2026.

Second order transport in two-dimensional electronic Fermi liquid

Pablo Reiser, Johannes Hofmann, Habib Rostami ¹University Of Bath, United Kingdom

Poster Session, Exhibition, Drinks Reception and Buffet, June 24, 2025, 17:30 - 19:30

We investigate the second-order (nonlinear) magnetotransport phenomena in a twodimensional electronic Fermi liquid in the presence of a sound-induced pseudogauge field by means of Landau kinetic theory. Our model explores the effect of the parity of the Fermi surface perturbation on the electron relaxation. This odd-even effect characterizes the "tomographic" regime, which can be to phenomenologically distinguish from the well-studied hydrodynamic and ballistic flows. In charged Fermi liquids, the long-range Coulomb coupling is treated by the introduction of screening of electron-electron interactions, limiting the range of the effective interaction to atomic size (short-range). We derive expressions for both the longitudinal and the transverse nonlinear conductivity and explore its relation with the field strength, cyclotron frequency and odd-even parity effects. Our results provide a theoretical framework for interpreting recent experimental observations of nonlinear magnetotransport.

Improved conductance and stability in Mo₂-based self-assembled monolayers through pyridine functionalisation

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Poster Session, Exhibition, Drinks Reception and Buffet, June 24, 2025, 17:30 - 19:30

We report the fabrication and characterisation of a novel set of Mo_2 -based compounds under ambient conditions. Through strategic molecular modification, we enhance the stability, assembly, and charge transport of these organometallic molecules, improving their suitability for molecular electronic and thermoelectric applications.

With the urgent need for sustainable energy solutions, thermoelectric energy harvesting has gained traction for reducing emissions and improving efficiency. A promising development in this field is the use of tailored organic thin films which can be engineered to exhibit advantageous quantum interference (QI) effects at room temperature[1]. These effects enhance thermal and electrical properties, making these films optimal candidates for thermoelectric energy harvesting.

This study focuses on three Mo_2 -based compounds $(Mo_2(INA)_4, Mo_2(D4PyF)_4)$, and $Mo_2(D3PyF)_4$, where $Mo_2(INA)_4$ is the base compound for synthesizing the modified isomers. While Mo_2 -integrated molecular junctions have shown promising thermoelectric performance[2], these specific compounds have not been previously explored as self-assembled monolayers (SAMs). The large planar structure and air sensitivity of $Mo_2(INA)_4$ present challenges for SAM fabrication, often leading to disordered assembly. However, the modified isomers offer improved stability, ease of handling, and potential for QI control.

SAMs were fabricated on template-stripped gold and characterised using AFM, XPS, and QCM. AFM confirmed monolayer formation with heights of ~1.5–2nm, aligning with theoretical predictions. Conductive AFM measurements of $Mo_2(D4PyF)_4$ and $Mo_2(D3PyF)_4$ revealed normalised log conductance values an order of magnitude greater than that of the unmodified $Mo_2(INA)_4$ SAM.

[1] X. Liu, et al. Angewandte Chemie, vol. 129, 2016.[2] M. Meng, et al. Nanoscale, vol. 12, 2020.

Massive interstitial strain and magnetic behaviour of the nickelate series Pr2-xCaxNiO4+ δ ($\delta >> 0$, $\delta \approx 0$)

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Poster Session, Exhibition, Drinks Reception and Buffet, June 24, 2025, 17:30 - 19:30

Layered perovskite oxides are well-known to host a myriad of electronic phases which are not fully understood, including unconventional superconductivity and charge density waves dependent on doping and temperature, often associated with distortions in the crystal structure as seen in tetragonal-to-orthorhombic phase transitions of certain cuprates. The neighbouring family of nickelates are a chemically similar yet relatively less explored family, also hosting strongly correlated behaviour such as striped charge and spin order in La2-xSrxNiO4 and high-temperature superconductivity under pressure in La3Ni2O7, giving this family potential to act as a Rosetta Stone of exotic condensed matter.

We have explored the ambient-pressure phase diagram of both $\delta >> 0$ and $\delta \approx 0$ Pr2xCaxNiO4+ δ using high-resolution powder X-ray diffraction, DC magnetometry and resistivity measurements, decomposing their structural evolution through irreducible representation (irrep) analysis with respect to the doped I4/mmm aristotype. The low-symmetry $\delta >> 0$ series evolves from C2/m -> Fmmm -> I4/mmm -> Fmmm symmetry upon doping; whereas the $\delta \approx 0$ series differently evolves from Bmab symmetry, consistently hosting massive orthorhombic Γ 4+ strain modes >2%, with X3+ displacive modes (irrep representing octahedral tilting) being symmetry-allowed in the $\delta \approx 0$ series but forbidden in the $\delta >> 0$ series. This is also reflected in magnetisation measurements showing a strong ZFCW-FCC splitting only in the former series, indicating a strong spin canting induced by the X3+ tilt mode (parameterising the Dzyaloshinskii-Moriya interaction) only upon loss of the interstitial oxygen, highlighting the importance of controlling oxygen content in designing strongly correlated nickelates.

Testing the putative Tomonaga-Luttinger liquid to Fermi liquid crossover in Li0.9Mo6017 through Boltzmann analysis of the Hall resistivity

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Poster Session, Exhibition, Drinks Reception and Buffet, June 24, 2025, 17:30 - 19:30

Li0.9Mo6017 (LMO) is a quasi-1D conductor and a strong candidate for realising a Tomonaga-Luttinger Liquid (TLL) as well as emergent symmetry. Its highly anisotropic resistivity hosts regimes of metallic, insulating and superconducting behaviour. Recent magnetoresistance (MR) and angle-dependent MR (ADMR) studies support both the emergent symmetry and TLL state in LMO. The ADMR data particularly have been interpreted as arising from dark excitons forming within the MoO chains at intermediate temperatures, responsible for both the resistive upturn below Tmin \approx 30 K and ultimately, the emergent symmetry. This claim relies on the TLL state remaining robust down to the superconducting transition temperature Tc \approx 2 K. It remains unclear, however, whether the response of the system is governed purely by TLL down to this temperature scale or whether it recovers higher-dimensional Fermi-Liquid (FL) behaviour in the regime Tc < T < Tmin.

To explore this issue, we apply Boltzmann transport theory (that would be inapplicable to a TLL) to model the field, temperature and angle dependence of the Hall resistivity $pxy(H, T, \vartheta)$ in LMO up to 35 T. Specifically, we apply the Ong construction in conjunction with the calculated Fermi surface of LMO and extract an anisotropic scattering rate that is itself field and temperature dependent. The ensuing parameterization is then mapped onto the model of dark excitons to test the viability of the model within a FL, rather than TLL, framework. The implications for a TLL-FL crossover and the nature of the ground state will then be discussed.

Electrically Tunable Femtosecond Dynamics of Excitonic Complexes in Single-Layer TMDs

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Poster Session, Exhibition, Drinks Reception and Buffet, June 24, 2025, 17:30 - 19:30

The two-dimensional nature of single-layer transition metal dichalcogenides (TMDs) leads to strong quantum confinement and reduced electrostatic screening, enabling the formation of tightly bound excitons and many-body excitonic complexes involving up to five particles and beyond. These complexes characterize the absorption and emission spectra of a vast number of semiconducting TMDs, and therefore understanding their response to optical excitation and other external stimuli is essential for optoelectronic applications. In this work, we employed femtosecond broadband pump-probe microscopy to investigate the dynamics of many-body excitonic complexes in single-layer WS2 and WSe2 under variable electrostatic doping via the field effect. Our transient spectra reveal signatures of trions, biexcitons and charged-biexcitons, providing insight into their ultrafast formation and decay processes. Most notably, we demonstrate control over the effective trion formation time across more than an order-of-magnitude, achieved with only moderate electron doping densities.

Improving the Precision of Thermoelectric Atomic Force Microscopy Measurements

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Poster Session, Exhibition, Drinks Reception and Buffet, June 24, 2025, 17:30 - 19:30

Thermoelectric devices are of interest for a number of practical applications, including miniaturised solid-state thermal management solutions and large-scale electrical harvesting of waste heat. Unfortunately, present thermoelectric devices suffer from low efficiency and power output compared to other heat-electricity conversion methods. In addition, many of the materials used in inorganic thermoelectric devices are toxic, scarce or harmful to the environment, limiting their potential for widespread implementation. Molecular electronics provides avenues towards improved thermoelectric performance by using quantum interference effects to control the properties of molecular-scale organic devices e.g., to enhance the Seebeck coefficient or suppress phonon transmission. In order to inform the design and development of future molecular thermoelectric devices, it is necessary to accurately measure key properties such as the electrical conductance, thermal conductance and Seebeck coefficient of candidate molecules.

In this work, a high-precision thermovoltage amplifier module which enables characterisation of the thermopower of molecular junctions formed by atomic force microscopy (AFM) has been developed. The key challenges of thermoelectric AFM measurements were identified, and corresponding design criteria established to ensure optimal performance. The resulting module can be constructed from inexpensive commercially available electronic components and 3D printed parts, and offers performance surpassing the best implementations reported to date.

Negative Intrinsic Viscosity in Graphene Suspensions: Insights from Molecular Dynamics and Continuum Theory

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Poster Session, Exhibition, Drinks Reception and Buffet, June 24, 2025, 17:30 - 19:30

The conventional wisdom in colloidal science holds that adding particles to a fluid increases its viscosity. However, graphene-based nanomaterials—owing to their atomic thickness and large lateral dimensions—exhibit rheological behavior that deviates significantly from classical hydrodynamic predictions. Using a combination of molecular dynamics (MD) simulations and continuum boundary integral (BI) theory, we investigated the shear viscosity of pristine graphene nanosheets suspended in water at high Péclet numbers. Contrary to expectations, we demonstrate that the intrinsic viscosity of the suspension can become negative when the graphene aspect ratio exceeds approximately 5.5.

MD simulations show excellent agreement with BI theory for slip particles across a range of aspect ratios (3-10), revealing that this anomalous behavior stems from two key factors. First, large hydrodynamic slip lengths at graphene surfaces significantly reduce viscous dissipation. Second, slip-induced torques stabilize the nanosheets in near-aligned configurations, minimizing rotational disruption of the flow field.

We compare quasi-two-dimensional and fully three-dimensional disc geometries in MD and find nearly identical viscosity trends, validating the quasi-2D approximation used in BI calculations. In both geometries, slip particles align with the flow direction, in stark contrast to no-slip particles, which exhibit tumbling motion characteristic of Jeffery orbits.

Finally, we examine concentration effects in semi-dilute regimes and identify an optimal solid fraction at which the effective viscosity reaches a minimum. This non-monotonic behavior is driven by interparticle interactions, which are more pronounced in no-slip systems. Our findings pave the way for ultra-low-viscosity 2D nanofluids, with applications in lubricants, conductive inks, and composites.

Scanned Andreev Tunnelling Microscopy: Atomic-scale visualisation of electronic structure and symmetry in spin-triplet superconductors

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Poster Session, Exhibition, Drinks Reception and Buffet, June 24, 2025, 17:30 - 19:30

Contemporary spectroscopic imaging scanning tunnelling microscopy (SI-STM) enlists a variety of single-particle tunnelling methods including shot noise measurements, electron-spin resonance, and standard lock-in spectroscopy. In the study of superconductors, two-particle tunnelling processes become accessible due to electron-hole hybridization. Notable among these methods is scanned Josephson tunnelling microscopy (SJTM) which directly probes the Cooper pair density in spin-singlet superconductors. However, a comparable probe of superconductivity in exotic spin-triplet superconductors and heavy fermions remains elusive. Here, by using a superconducting Nb scan tip, we introduce Scanned Andreev Tunnelling Microscopy and Spectroscopy (SATM) which has provided significant insights into the spintriplet superconductor UTe₂. Measurements performed on the (0 -1 1) surface of UTe₂ reveal the presence of an Andreev bound state. Measuring the Andreev conductance to this bound state across an adsorbed metallic cluster confirms that the zero-energy bound state is a direct consequence of bulk superconductivity. Next, spectroscopic and junction dependent measurements reveal that this zero-energy conductance arises predominantly from Andreev tunnelling processes, with negligible contribution from the Josephson effect, and that this conductance is the result of resonant Andreev reflection at zero-energy. Furthermore, the superconducting tunnel junctions used herein lead to multiple Andreev reflections. We introduce these combined SATM measurements and demonstrate that they represent a promising pathway to directly measure and visualise at the atomic scale the superconducting energy gap, pair density waves, and quasiparticle surface bands in spin-triplet and heavy fermion superconductors.

Simulating 23Na NMR of sodium-ion-modified ZIF-62 glass

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Poster Session, Exhibition, Drinks Reception and Buffet, June 24, 2025, 17:30 - 19:30

ZIF-62 is a mixed-linker metal-organic framework known for its exceptionally high glass-forming ability. Taking inspiration from silicate-based glass techniques, modifying glassy ZIF-62 with Na+ substantially lowers its glass transition temperature, which promises to improve its overall processability[1]. Here, we simulated 23Na NMR via DFT GIPAW on Na+-ZIF-62 to determine the mechanisms responsible for its decreased transition temperature. 200 Na+ environments were generated and classified according to their match with experimental NMR spectra. We found Na+ substitution in ZIF-62 distorts the framework and reduces connectivity, leading to 4- or 3-coordinated Na+. This contrasts the 6- or 5- coordinated Na+ in Na+-modified silicate glasses. The unique structural role of Na+ in Na+-modified ZIFs highlights the potential to adapt glass modification principles to MOF-based systems, achieving new structural and functional outcomes.

FaRMS: Facility for Radioactive Materials Surfaces

<u>Chris Bell</u>¹, L. Harding¹, R.S. Springell¹ ¹University of Bristol, United Kingdom

Poster Session, Exhibition, Drinks Reception and Buffet, June 24, 2025, 17:30 - 19:30

Funded by the EPSRC National Nuclear User Facility (NNUF), this Facility, based at the University of Bristol, hosts a thin film growth system capable of fabricating high quality active thin films and surfaces for fundamental and applied studies [1]. This system is complemented with an X-ray Photoemission Spectroscopy (XPS) system enabling surface analysis and depth-profiling. Users can engineer samples, from idealised single crystal model systems, to more complex, multi-element, granular structures that more closely represent the real world. The properties of thin film samples are dominated by surface/interfacial effects, and hence are ideal to understand phenomena such as oxidation, dissolution, pitting, cracking, species migration, hydriding and interaction with water, which are of crucial importance across the nuclear sector. A key aspect of this Facility is that typically, sample activity will range from 0.1 – 10 Bq/g, which means that samples can be easily accepted into universities and national facilities that do not currently have licenses for large quantities of active material. A recent review of several decades of work associated with this system can be found in Ref. [2]. References

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Mapping Pressure to Doping in Optimally Doped YBa2Cu3O6+x

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Poster Session, Exhibition, Drinks Reception and Buffet, June 24, 2025, 17:30 - 19:30

The unconventional superconducting behaviour of cuprates is remarkable in several respects, most notably in their high critical temperatures at ambient pressure. In YBa2Cu3O6+x (Y123), the primary method used to tune Tc is hole doping into the CuO2 planes, typically achieved by variation of oxygen content in the copper oxide chains. However, studies have shown that pressure can be used as an alternative tuning parameter for Tc by increasing the overlap of orbitals.

In this work, we address the question of whether the relationship between doping and pressure is direct. We perform DC magnetisation measurements in diamond anvil cells (DACs) to determine Tc as a function of pressure. We use background subtraction to isolate the signal produced by a sample in its superconducting state from the contribution of the DAC. Up to 20 GPa in optimally doped Y123, we observe a reduction in Tc which is consistent with a single scaling parameter that maps pressure onto doping. Our findings are in agreement with earlier work by Alireza et al. [1] which focuses on over-doped samples.

[1] Alireza et al., Accessing the entire overdoped regime in pristine YBa2Cu3O6+x by application of pressure. Phys. Rev. B, 95, 100505(R). 2017.

Condensed Matter and Quantum Materials 2025

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