Wagga2026/AC2MP2026

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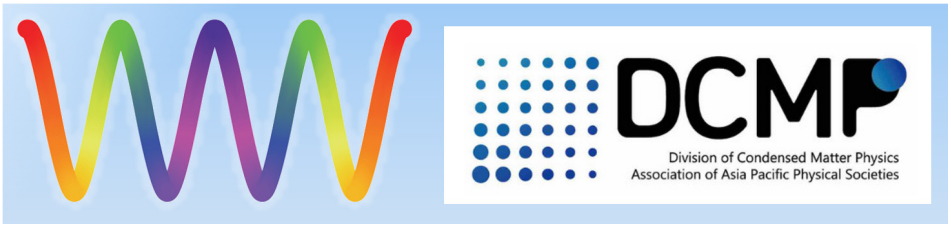
Charles Sturt University, Wagga Wagga NSW Australia



Book of Abstracts

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Topological materials / **8**

Non-equilibrium orbital dynamics in Bloch electron systems

Author: Dimi Culcer[1]

Co-authors: Hong Liu [1]; James Cullen [1]; Rhonald Burgos [1]

[1] *UNSW Sydney*

In this talk I will discuss a series of insights into non-equilibrium phenomena involving the orbital angular momentum (OAM) of Bloch electron systems. Recent years have witnessed a surge of interest in the orbital angular momentum of Bloch electrons, motivated by its emerging applications in spintronics and magnetic memory [1]. I will first show that disorder plays a crucial role in the orbital Hall effect, at least when the OAM current is evaluated according to the conventional prescription of multiplying the matrix elements of the OAM by those of the velocity [2]. Building on this insight I will show that, more importantly, the conventional evaluation of the orbital Hall effect suffers from a fundamental flaw. Evaluations of the orbital Hall effect have only retained inter-band matrix elements of the position operator. I will outline the correct way to evaluate the OHE including all matrix elements of the position operator, including the technically challenging intra-band elements [3]. They also give rise to a giant OHE in the bulk states of topological insulators, which greatly exceeds spin-related effects [4]. Finally I will discuss our recent insights into the orbital magneto-electric effect. I will show that the OME is partly the result of a non-equilibrium dipole moment generated via Zitterbewegung and proportional to the quantum metric. Our results suggest quantum metric engineering as a route towards maximizing orbital torques [5]. In closing I will give an overview of outstanding questions in the field which include the full role of disorder, inhomogeneities, and the non-conservation of the OAM due to intrinsic mechanisms, which our group has also identified [6].

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Field of Condensed Matter:

Theory

Thermo- and magneto-electrics / **9**

Quantum geometry and dipolar dynamics in the orbital magneto-electric effect

Author: James Cullen[1]

Co-author: Dimi Culcer [2]

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Recent years have seen a dramatic surge of interest in the field of *orbitronics*, which looks to harness the orbital angular momentum of electrons in computing devices. Orbitronic devices require the efficient generation of orbital angular momentum densities or currents. In this work we derive expressions for the orbital magneto-electric effect – the electrical generation of a steady-state orbital angular momentum density – in Bloch electrons, tracing each contribution back to distinct physical mechanisms. We show that the orbital magneto-electric effect is partly the result of a nonequilibrium dipole moment generated via Zitterbewegung and proportional to the quantum metric. For tilted Dirac fermions this dipole gives the *only* contribution to the orbital magneto-electric effect, while the intrinsic and extrinsic contributions are nonzero for different electric field orientations, yielding an experimental detection method. Additionally, the dipole density can be nonzero in the insulating gap, providing a physical reason for the orbital magneto-electric effect to be nonzero in the gap. Our results suggest quantum metric engineering as a route towards the efficient generation of orbital angular momentum.

Field of Condensed Matter:

Theory

Superconductivity / **10**

Topological Superconductivity in an atomic Sn layer on a semiconductor substrate

Author: Stephan Rachel[None]

A third monolayer of tin atoms on the semiconductor substrate Si(111) has been shown to become superconducting upon six to ten percent hole doping. Experiments have reported promising results hinting at a superconducting chiral d-wave order parameter [1]. Here we examine Sn/Si(111) by combining most recent ab initio results, quasi-particle interference calculations, state-of-the-art truncated-unity functional renormalization group simulations and Bogoliubov-de Gennes analysis. We show remarkable agreement between experimental and theoretical quasi-particle interference data both in the metallic and superconducting regimes. The interacting phase diagram reveals that the superconductivity is indeed chiral d-wave with Chern number C=4. Surprisingly, magnetically ordered phases are absent, instead we find charge density wave order as seen in related compounds. We extend our analysis to the related compounds Pb/Si(111), Sn/SiC(0001) and Pb/SiC(0001), which exhibit different strengths of spin-orbit coupling and different interaction strength. Our results suggest that also these materials are promising candidate materials for chiral topological superconductivity.

[1] F.Ming, *et int.*, H.H. Weitering, Nat. Phys. **19**, 500 (2023).

Field of Condensed Matter:

Superconductivity

Materials under extreme conditions / **12**

Compact Pulsed Magnetic Field for Quantum Beam Experiments

Author: Hiroyuki NOJIRI[1]

[1] *Institute for Materials Research, Tohoku University*

Recently, the installation of a pulsed magnet has brought a new breakthrough in x-ray experiments in high magnetic fields. It expands the magnetic field range from 10-15 Tesla to 30-50 Tesla. In such strong magnetic fields, the effect of a magnetic field is not a weak perturbation but is a cause of the in-trinsic and significant phenomena in many cases. We report recent progresses in high magnetic field X-ray experiments with SR and XFEL sources.
The observation of weak super-lattice peaks caused by electronic transi-tions such as CDW, Fermi surface nesting and others is very difficult in SR source. The breakthrough has been made by the combination of the high intense XFEL beam and the single shot pulsed field. A tiny CDW peaks in YBCO have been observed successfully in a single short diffraction. It will extend the application of pulsed field x-ray diffraction for systems with weak spin-charge-lattice couplings.
In this presentation, the technical developments, recent examples of experiments, and the future development such as resonant scattering will be presented. The application for neutron diffraction and THz spectroscopy will be also explained.

Field of Condensed Matter:

Quantum Materials

Superconductivity / **13**

Unconventional Magnetism and Nonreciprocal Superconductivity

Author: GiBaik Sim[1]

Co-author: Stephan Rachel

[1] *The University of Melbourne*

Magnetic systems with momentum-dependent spin splitting provide fertile ground for discovering unconventional phases of matter beyond conventional ferromagnetism and antiferromagnetism.

The recently identified p-wave magnet represents a new class of magnetic order exhibiting odd-parity, time-reversal-symmetric spin splitting in momentum space, offering a promising platform for spintronic applications. We establish a microscopic interacting model that realizes the p-wave magnet as its ground state: starting from a Hubbard model, we derive the low-energy spin Hamiltonian and show that quantum order-by-disorder lifts the classical degeneracy and stabilizes the p-wave magnet. The resulting band structure exhibits finite spin accumulation via the Edelstein effect, highlighting its spintronic applications.[1]

Based on the symmetry principle, we further show that the momentum-dependent spin splitting in metallic altermagnets (d-wave magnets) naturally induces pair-density-wave superconductivity even in the absence of magnetic fields. Within a BCS framework, we identify Fulde–Ferrell and Fulde–Ferrell* states that spontaneously break inversion symmetry and exhibit nonreciprocal supercurrents, giving rise to a supercurrent diode effect.[2]

[1] Sim, G., & Rachel, S. (2025), ArXiv preprint arXiv:25xx.xxxxx
[2] Sim, G., & Knolle, J. (2025), Physical Review B, 112(2), L020502.

Field of Condensed Matter:

Theory

Topological materials / **14**

Hopfions in Condensed Matter: Anisotropic Heisenberg Magnets

Author: Avadh Saxena[1]

[1] *Los Alamos National Lab*

Nontrivial topological defects such as knotted solitons called hopfions have been observed in a variety of materials including chiral magnets, nematic liquid crystals and even in ferroelectrics as well as studied in other physical contexts such as Bose-Einstein condensates. These topological entities can be modeled using the relevant physical variable, e.g., magnetization, polarization or the director field. Specifically, we find exact static soliton solutions for the unit spin vector field of an inhomogeneous, anisotropic three-dimensional (3D) Heisenberg ferromagnet and calculate the corresponding Hopf invariant H analytically and obtain an integer, demonstrating that these solitons are indeed hopfions [1]. The invariant H is a product of two integers, the first being the usual winding number of a skyrmion in two dimensions, while the second integer encodes the periodicity in the third dimension. We also study the underlying geometry of H, by mapping the 3D unit vector field to tangent vectors of three appropriately defined space curves. Our analysis shows that a certain intrinsic twist is necessary to yield a nontrivial topological invariant, i.e., a linking number [2]. We also focus on the formation energy of hopfions to study their properties for potential applications. Finally, we investigate the dynamics of hopfions interacting with an array of line defects resulting in a toron under certain conditions. In addition, we find that an asymmetric array of defects leads to a hopfion ratchet effect [3].

[1] R. Balakrishnan, R. Dandoloff, and A. Saxena, Phys. Lett. A 480 128975 (2023).
[2] R. Balakrishnan, R. Dandoloff and A. Saxena, Phys. Lett. A 493, 129261 (2024).
[3] J.C.B. Souza et al., Scientific Reports 15, 16802 (2025).

Field of Condensed Matter:

Magnetism

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Inelastic neutron scattering and novel magnetic materials

Author: Dehong Yu[1]

[1] *Australian Nuclear Science and Technology Organisation*

Neutrons are fundamental particles that form atoms and, consequently, matter. The unique properties of thermal neutrons make them a powerful tool for characterizing and investigating various materials at the atomic scale. The wavelength and energy of thermal neutrons are comparable to the structural scale and the energy of elementary excitations in matter. Inelastic neutron scattering can probe the dynamic properties of atoms and reveal correlations between dynamics and structure—i.e., the time and space correlations essential for a fundamental understanding of material properties. Additionally, neutron spin can directly reveal the spin structure and dynamics in novel magnetic materials.

In this presentation, I will demonstrate how inelastic neutron scattering provides a deep understanding of spin dynamics in quantum magnets, using several case studies performed on the PELICAN time-of-flight neutron spectrometer at ANSTO [1]. These studies include realisation of 2D quantum universality in the triangular-lattice quantum antiferromagnet Na2BaCo(PO4)2 [2]; observation of the magnetic structure phase transition in the honeycomb antiferromagnet Na3Ni2BiO6 [3]; and confirmation of the two-magnon bound state Bose-Einstein condensation of spin-1 triangular lattice [4].

References:

[1] D.H. Yu, et al. J. Phys. Soc. Jpn. 2013, 82, SA027.
[2] J.M. Sheng, et al. Proceedings of the National Academy of Sciences (PNAS). 2022, 119, e2211193119.
[3] Y. Shangguan, et al. Nature Physics, 2023, s41567-023-02212-2.
[4] J.M. Sheng, et al., Nature Materials, 2025, 24, 544-551.

Field of Condensed Matter:

Magnetism

Magnetism / **16**

Revealing triclinic symmetry and magnetic properties of YCrO3 Perovskites

Author: Hai-Feng Li[1]

[1] *University of Macau*

This research delves into the triclinic symmetry and ferroelectric nature of YCrO3, a chromium-based perovskite, using single-crystal neutron diffraction. We uncover a unique structural configuration that accounts for its ferroelectric properties, alongside a G-type antiferromagnetic arrangement. The study provides a comprehensive analysis of the interplay between lattice and spin degrees of freedom, offering valuable insights into the coexistence of magnetic and electric orders. These findings enhance our understanding of YCrO3's potential in multifunctional applications, emphasizing the critical role of precise structural investigations in advancing perovskite research.

Field of Condensed Matter:

Magnetism

Condensed matter theory / **17**

Materials structures and their properties through self-consistent computational simulations and comparisons in quantitative convergent beam electron diffraction measurements.

Author: Andrew E. Smith[None]

Co-authors: Muhammad Owais ; Loreibelle Abian ; Bikas Aryal ; Mostafa Eid ; Laure Bourgeois ; Philip N. H. Nakashima

Comparisons of calculated electron density distributions within self-consistent Density Functional Theory (DFT) are made with those of experimental results, determined from Quantitative Convergent Beam Electron Diffraction (QCBED).

Use of the WIEN2k [1] computational package, based on LAPW + lo , enables simulation of bonding electron densities comparable with those determined from QCBED experiments, potentially using a nano-sized probe. Through scattering theory, the Fourier transform of the material electron density is related to the X-ray scattering factor, which in turn relates to the high energy electron scattering by means of the Mott-Bethe formula. The single indicative computational parameter chosen for WIEN2k is RKmax, the product of the muffin tin radius with the maximum k vector value. In contrast DFT methods such as VASP [2], based on plane wave expansions, employ an energy cut off parameter Ecut together with maximum k vector value.

Earlier work on aluminium using the Wien2k approach was in very close agreement with a benchmark QCBED study and demonstrated how simulations for structures and properties were improved by more careful computational parameter choice in comparison with literature computational simulations of XRD analysis using less rigorous parameters [3]. Recently, work on aluminium and its voids has demonstrated how the careful use of the RKmax parameter has enabled calculations to be carried out within a reasonable time and be sufficiently efficient for large super cells containing multiple vacancies [4].

In particular, we have used enhancements of WIEN2k which provide a more effective use of computational precision switches principally dealing with states close to the Fermi level, i.e. whether the material is metallic, insulator or semi-conductor. They have more efficient predictions of the lattice parameter for aluminium [4].

Our recent work has not only dealt with aluminium and its alloys, but also such materials as the perovskites SrTiO3 and KTaO3 [5], together with layered ZnInO structures, TiO2 and Mg3Sb2.

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Field of Condensed Matter:

Theory

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The Magnetic Ground State of Atacamite Cu2Cl(OH)3: The Crucial Role of Frustrated Zigzag Chains Revealed by Inelastic Neutron Scattering

Authors: Jackson Allen[1]; Kirrily Rule[None]

Co-authors: Leonie Heinze [2]; Oleg Janson [3]; Richard Mole [4]; Roger Lewis ; Satoshi Nishimoto [5]; Stefan Suellow [6]

[1] *University of Wollongong*

[2] *JCNS*

[3] *Institute for Theoretical Solid State Physics, Leibniz Institute for Solid State and Materials Research Dresden*

[4] *ANSTO*

[5] *TU Dresden*

[6] *TU Braunschweig*

We report inelastic neutron scattering (INS) measurements on the magnetically frustrated S = 1/2 sawtooth-chain compound atacamite Cu2Cl(OH)3 featuring inequivalent Cu(1) and Cu(2) sites. Transverse to the sawtooth chains, INS reveals two dispersive spin-wave modes and a gap of at least 0.75 meV. This behaviour is rationalized within a zigzag-chain model of Cu(2) spins in an effective magnetic field of Cu(1) spins. The model is compatible with first-principles calculations and accounts for INS dispersions within linear spin-wave theory calculations. Our results reveal a unique case of an effective separation of energy scales between two differently oriented one-dimensional chains, with the zigzag-chain model being essential to fully characterize atacamite's low-energy magnetism.

Field of Condensed Matter:

Magnetism

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Phonon Softening Anomalies and Phase Transformations

Author: Trevor Finlayson[1]

Co-authors: Hanus Seiner ; Kirrily Rule [2]

[1] *University of Melbourne*

[2] *ANSTO*

The term "soft phonon mode"was first introduced by Cochran in describing the lattice dynamical behaviour for certain ferroelectric crystals [1]. Within the past forty years or so, the term has been applied, perhaps somewhat loosely, to describe almost any section of a phonon dispersion relation for which frequency decreases as temperature decreases. So the real relationship between "phonon softening anomalies"and "phase transformations"has been a point of confusion in the literature, as was discussed some years ago by Professor Jim Krumhansl [2].

In this presentation, I shall review some of the observations of anomalous phonon softening and the extent to which such features of the lattice dynamics, relate to a phase transformation of the crystal of interest. Such transformations range from a quite simple cubic to tetragonal transformation involving an associated softening of low-q, acoustic phonons, as in the A-15 structure compound, V3Si, [3] to the more complex structural changes resulting in modulated structures related to phonon anomalies at specific values of q along a dispersion relation, as in the magnetic shape memory Ni-Mn-Ga alloys [4].

In our own recent research on In-Tl alloys which exhibit a cubic to tetragonal transformation on cooling [5], which old literature attributed to a low-q phonon anomaly on the T2 branch [6], there is no phonon softening along this branch [7]. Rather, a slight phonon softening of the [111]T zone-boundary phonon with decreasing temperature [8] was suggested to be consistent with a transformation mechanism involving defect formation on {111} conjugate crystal planes connecting the cubic and tetragonal crystal structures [9].

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Field of Condensed Matter:

Magnetism

Topological materials / **22**

Accuracy of Majorana braids as quantum gates in the face of disorder

Authors: Cole Peeters[None]; Themba Hodge[1]; Eric Mascot[1]; Stephan Rachel[1]

[1] *Melbourne Uni*

Recently, there has been a great deal of interest in topological quantum computing as a means of circumventing many common sources of errors present in traditional quantum computers. In particular, semiconductor-superconductor heterostructures, quantum dot-superconductor arrays, and magnet-superconductor hybrid systems are all being investigated for their ability to host Majorana zero modes (MZMs): non-Abelian anyons [1] which have the theoretical ability to encode quantum Clifford gates whose accuracy is guaranteed by their topological nature.
In this talk I will discuss recent work we have done which examines the robustness of this topological protection, especially in the face of impurities and disorder which are expected to be present in most physical systems [2]. By simulating the full time-dependent exchange of MZMs on a T-junction geometry constructed from Kitaev chains, we are able to quantify the error introduced by localized impurities, finding that it agrees with low energy analytics. We also consider the ability for the presence of disorder to stabilize the topological phase, potentially reducing the gate error compared to the perfectly clean system.

[1] C. Nayak, et al. Non-Abelian anyons and topological quantum computation. Rev. Mod. Phys. 80, 1083–1159 (2008).
[2] C. Peeters, et al. Effect of impurities and disorder on the braiding dynamics of Majorana zero modes. Phys. Rev. B 110, 214506 (2024); Editors' suggestion

Field of Condensed Matter:

Topological Materials

Superconductivity / **23**

Exotic superconductivity in time-reversal symmetry broken honeycomb systems

Authors: Lucca Marchetti[1]; Matthew Bunney[2]; Stephan Rachel[1]

[1] *University of Melbourne*

[2] *University of Melbourne, RWTH Aachen University*

Rhombohedral graphene –stacked graphene layers in the ABC configuration –has emerged as an exciting playground for strongly correlated physics and superconductivity. Recent experiments on N-layer rhombohedral graphene reveal signatures of spontaneous time reversal symmetry breaking as well as spin-valley polarised Fermi surfaces. Probes at low temperature reveal several regions of superconductivity, with signs of chiral triplet pairing states [1–3]. To better discern how broken symmetries in the normal state affect underlying many-body states we focus on 2D single-layer honeycomb systems in the presence of various symmetry breaking terms. We employ the truncated-unity functional renormalisation group technique to analyse the leading instabilities of the associated Hubbard model, which takes a microscopic model and interpolates between the bare Hubbard interaction and a low-energy two-particle interaction vertex. We discuss how the different broken symmetries affect the resulting superconductivity, and the implications this has for chiral and/or triplet pairing states. We further characterise the superconducting states in a topological context through calculation of Chern number landscapes, where we find regions of topological superconductivity.

References:
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Field of Condensed Matter:

Superconductivity

Condensed matter theory / **24**

Computations on Calcite

Author: Christopher Howard[1]

Co-authors: Boyuan Gou [2]; Ding Xiangdong [2]; Ekhard K.H. Salje [3]; Jun Sun [2]; Yang Yang [2]; Yixin Lin [2]

[1] *University of Newcastle, Australia*

[2] *State Key Laboratory for Mechanical Behaviour of Materials, Xi'an Jiaotong University, China*

[3] *Department of Earth Sciences, University of Cambridge*

The crystal structure of calcite, CaCO3 at room temperature was examined in the early days of crystallography (Bragg, 1914). A phase transition at around 1240 K was also reported (Boeke 1912). But experimental studies at higher temperature are problematic because calcite starts to decompose at around 1100 K.

We have used computation, specifically molecular dynamics (MD), to explore behaviour at higher temperatures (Yang et al., 2025a). Above about 2000 K the CO3 entities that at room temperature lie in planes re-orient to become effectively spherical, and the structure reduces to the halite structure, cubic, in space group Fm-3m. There is a phase transition around 2000 K, below which the CO3 develop a tendency to lie in a particular plane but are disordered with this plane –the structure is described in space group R-3m. There is another transition computed to be at 1525 K, corresponding to the transition reported to occur at 1240 K, to the known room temperature structure. This has the CO3 lying in planes and ordered within these planes, the CO3 orientation reversing between one plane and the next. The space group is R-3c and on account of the reversals just mentioned the repeat is twice that in R-3m.

We have considered the order parameters for these two transitions. The coupling between them is linear-quadratic, and the interaction between them will be reported. We have also made a detailed study of twinning in calcite (Yang et al., 2025b).

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Boeke, H.E. Neues Jaahrb Miner. 1, 91-121, 1912.

Yang, Y. et al., Phys. Chem. Miner. 52,7, 2025.

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Field of Condensed Matter:

Theory

Spectroscopies 1 / **26**

Nonlinear Absorption in Perovskite Materials

Author: David Ompong[None]

Co-authors: Daniel Dodzi Yao Setsoafia [1]; Emmanuel Ofosu ; Hooman Mehdizadeh- Rad [1]; Jai Singh [1]; Kiran Sreedhar Ram [1]; Michael Edem Donkor

[1] *Charles Darwin University*

Optical absorption is of paramount importance for any material that is used in photovoltaic, lasing, light emitting diodes, etc., applications. Perovskite materials have several potential nonlinear optical applications. A thorough understanding of two-photon absorption (TPA) in perovskite semiconductors is required for nonlinear optical applications [1-4]. We have derived a TPA coefficient K2 for perovskite semiconductors using second-order perturbation theory and within the parabolic-band approximation, including excitonic effects. The derived K2 has Egˆ3/2 dependence and shows that perovskite semiconductors exhibit allowed-forbidden two-photon transitions. We have found that in perovskite materials, the increasing bandgap with temperature contributes to an increase in K2 from 290 K to 50 K [5], which is contrary to the TPA coefficient behaviour in most tetrahedral semiconductors. There is a satisfactory agreement between the theoretical and the experimental TPA coefficients at 290 K and 50 K. Our study highlights the importance of including excitonic and relativistic effects when considering TPA spectra in perovskite semiconductors.

Field of Condensed Matter:

Energy and Functional Materials

Topological materials / **27**

Transfer Matrix Approach for Topological Edge States

Author: Rickson Wielian[1]

Co-authors: Ivan Toftul [1]; Yuri Kivshar [1]

[1] *Australian National University*

We suggest and present an approach for describing the topological properties of a periodic system from the transfer matrix associated with a unit cell. This way, each Hamiltonian is mapped to a curve in the space of transfer matrices. The winding of the curve in this space is then associated to the existence of topological edge state. We use the Iwasawa decomposition to parametrize the transfer matrix uniquely in terms of three real numbers. This allows us to obtain simple analytical conditions for the existence of topologically protected edge states and to provide a visual illustration of all possible solutions. To demonstrate our method, we also apply it to study some generalizations of the Su-Schrieffer-Heeger (SSH) model, such as the tetramer SSH4 model and a one-dimensional photonic crystal inspired by the SSH model. Finally, we also show a simple pictorial proof of the Zak phase bulk-edge correspondence for any inversion-symmetric one-dimensional system using this approach.

Field of Condensed Matter:

Topological Materials

Condensed matter theory / **28**

Cavity Quantum Materials — The rise of vacuumronics

Author: Qing-Dong Jiang[1]

[1] *Shanghai Jiao Tong University*

Controlling quantum states of matter on demand is a cornerstone of emerging quantum technologies. In this talk, I will present an alternative to the conventional and fruitful use of electromagnetic radiation—which often leads to heating and nonequilibrium dynamics—by instead harnessing quantum fluctuations themselves as a tool to probe and manipulate quantum matter. Specifically, I will

discuss how vacuum fluctuations, when combined with symmetry breaking, give rise to a variety of striking phenomena, including the quantum atmospheric effect and vacuum–cavity–induced modifications of band structures, topology, and magnetism in quantum materials.

Field of Condensed Matter:

Quantum Materials

Condensed matter theory / **29**

A Unified Quantum-Geometric Framework for Generalized Artificial Neural Networks

Author: Muhammad Nawaf Nafi[1]

[1] *Bangladesh Air Force Shaheen College Dhaka*

We present a unified framework integrating Loop Quantum Gravity (LQG) and Quantum Field Theory (QFT) to model abstract Artificial Neural Networks (ANNs). Existing ANNs lack a physical basis for higher-order cognition, self-reference and general intelligence, motivating an LQG- and QFT-based framework. We model neurons as quanta of space at LQG spin-network nodes, neuron states as quantum states in Hilbert space and edges labeled by spins serving as complex spin-weights defining the network topology. Information processing is described as quantum-state evolution governed by Hamiltonian constraints of LQG, where learning consists of discrete, unitary, energy-conserving updates, reducing curvature and encoding information as geometric deformation. QFT-based input and output layers are modeled as continuous field excitations that interact coherently with the discrete spin-network geometry. Spin transitions yield gradient-like updates linking optimization to curvature flow in quantum geometry. Higher-order dynamical feedback states emerge that encode both external data and the network's own evolution, enabling self-referential computation. Conserved excitations interacting as particles in QFT drive the unitary evolution that sustains memory, suggesting a unified ANN framework.

Field of Condensed Matter:

Theory

Magnetism / **31**

Standard model of electromagnetism in crystals: Multipole order and beyond

Authors: Roland Winkler[1]; Ulrich Zuelicke[2]

[1] *Northern Illinois University*

[2] *Victoria University of Wellington*

Quantum materials exhibit a plethora of novel electric and magnetic orders beyond the textbook examples of ferroelectrics and ferromagnets. These include multiferroics [1], altermagnets [2], and novel forms of chirality [3]. The richness of materials and phenomena is reminiscent of mid-last-century particle physics, when a confounding zoo of "elementary" particles was only systematically understood after the standard model became established.

We have developed a standard model of electric and magnetic order in crystalline solids that provides a physically transparent, unified framework for the multitude of quantum materials [4,5]. Symmetry is its guiding principle. A formal analogy between space inversion and time inversion is used to identify two complementary, comprehensive classifications of crystals, based on five categories of electric and magnetic multipole order ("polarizations") and five categories of chirality. Jointly, the categories of polarizations and chirality yield a classification of all 122 magnetic crystal classes into 12 types that exhibit distinct physical properties. The 12-type classification also reveals striking correspondences between apparently dissimilar systems.

The standard model has predictive power by relating electric and magnetic multipolar order with the electronic band structure as well as property and response tensors, in the process enabling the absolute quantification of electric and magnetic multipole order [6].

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Field of Condensed Matter:

Quantum Materials

Materials and devices / **32**

A Computational Investigation into Hydrogen Production on Twisted Molybdenum Disulfide

Author: Kayla Prendergast[1]

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Hydrogen is a promising zero-carbon fuel which can be formed using renewable electricity, and when utilising electrolysis the most effective catalysts found so far are all platinum based. Given platinum is a rare and expensive metal, attention has shifted to transition metal dichalcogenides, such as monolayer (2D) MoS2, which are earth abundant and show promising catalytic activity. While currently less effective than platinum-based catalysts, the activity of MoS2 has proven to be highly tuneable by introducing dopants,[1] defects,[2] and supporting materials,[3] which modify the geometric and electronic structure.

Very recently, changes in the electronic structure of layered 2D materials have been observed when the layers are twisted relative to each other, giving rise to the emerging field of twistronics. Despite growing interest in the topic, little is known about how a twist in supported MoS2 might affect its catalytic activity in the hydrogen evolution reaction. This work involved a systematic computational study using density functional theory to calculate the hydrogen evolution activity of twisted, layered MoS2. This allowed for the effects of twist angles on various systems to be isolated and examined.

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Field of Condensed Matter:

Energy and Functional Materials

Magnetism / **33**

Using applied magnetic fields to induce unconventional magnetic order in the frustrated quantum magnet, clinoatacamite, Cu2Cl(OH)3

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The natural mineral clinoatacamite, $[Cu_2Cl(OH)_3]$, exhibits low-temperature, frustrated magnetic behaviour where competing interactions are responsible for novel magnetic properties. Attempts to establish the magnetic phases in this material have been undertaken and an unconventional applied field (H||b) phase diagram has been revealed. Two critical transition temperatures at zero field have been identified with long range antiferromagnetic (AFM) order for T_1 < 6K, and paramagnetic behaviour for T_2 >18K. In-field magnetisation data collected between 6-18K reveal three distinct phases for H||b which are not completely understood. Until now, the phase diagram of clinoatacamite has not been probed for H||a*or H//c*. We will present neutron scattering measurements of single crystal clinoatacamite in applied fields up to 10T. With these measurements we have mapped out the phase diagram of the antiferromagnetic structure for H||a*.

Field of Condensed Matter:

Magnetism

Amorphous / non-crystalline materials / **35**

Formation of Intermetallic Compounds: A Liquid Structure Perspective

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Rare earth elements are commonly incorporated into aluminum alloys to refine grains and enhance mechanical properties through forming the intermetallic compounds. However, the atomic-level mechanism governing the formation of these compounds during solidification remains insufficiently understood. In this work, Al-Cu and Al-Cu-La liquid alloys were investigated using synchrotron high-energy X-ray diffraction, ab initio molecular dynamics and reverse Monte Carlo simulations.

The solute–solvent interactions and atomic structure of both liquid alloys were analyzed and compared. The results reveal a strong affinity between Al and La atoms, and minor La addition significantly enhances icosahedral order in the Al-Cu liquid. Furthermore, the local atomic arrangement in the Al-Cu-La liquid closely resembles that of the $Al_{11}La_3$ crystal, providing favorable structural conditions for the nucleation of $Al_{11}La_3$ phase. These findings demonstrate the structural role of La in Al-Cu liquids and provide deeper insights into the formation of $Al_{11}La_3$ intermetallic compound.

Field of Condensed Matter:

Noncrystalline materials and physics

Magnetism / **37**

Fractal Path DMRG on the Triangular Antiferromagnet

Author: Oliver Bellwood[1]

[1] *Okinawa Institute of Science and Technology Graduate University*

The area law of entanglement entropy is known to heavily constrain the accessible system sizes in tensor network method simulations of 2D quantum magnetism. The situation is further complicated by the presence of geometrical frustration, which enhances quantum fluctuations and ground state degeneracy, leading to increased computational difficulty. We recently demonstrated that the Density Matrix Renormalization Group algorithm is enhanced by a judicious choice of the bijective mapping for the Matrix Product State ansatz of the square lattice antiferromagnet [1]. In particular, we showed that any fractal path mapping, such as the Hilbert curve, improves convergence of the algorithm with respect to bond dimension over the conventional row-by-row mapping. We show that such convergence enhancement is also seen for the triangular antiferromagnet, allowing for accurate determination of the ground state energy and magnetization.

[1] arXiv:2507.11820

Field of Condensed Matter:

Magnetism

Topological materials / **38**

Prediction of quantum spin Hall and Rashba effects in two-dimensional Pristine and Janus Ag-doped $AuBiO_3$ Monolayers

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Co-authors: Aniceto B. Maghirang III [1]; Chia-Hsiu Hsu [2]; Feng-Chuan Chuang [1]; Gennevieve M. Macam [3]; Guo-qing Chang [2]; Rovi Angelo B. Villaos [1]; Zhi-Quan Huang [1]

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Two-dimensional oxides are gaining attention as promising materials for investigating quantum and spin-related phenomena. In this research, we analyse both pristine $AuBiO_3$ and its Janus variant with Ag doping ($Au_{0.5}Ag_{0.5}BiO_3$) by employing first-principles density functional theory using PBE (Perdew-Burke-Ernzerhof) and hybrid functional (HSE06) calculations. The incorporation of Ag atoms at the A-site disrupts inversion symmetry, resulting in a Janus structure that boosts spin–orbit coupling (SOC) and alters the electronic and topological characteristics of the material.

The phonon dispersion and total energy analyses verify that both monolayers exhibit stability both dynamically and thermodynamically. The pristine $AuBiO_3$ monolayer shows an indirect bandgap that emerges under SOC, leading to a quantum spin Hall (QSH) insulating phase with a non-trivial topological invariant ($Z_2 = 1$) and gapless helical edge states. Notably, the Janus Ag-doped $AuBiO_3$ maintains the QSH state but presents a larger bandgap of approximately 0.33 eV, as calculated with the HSE06 method.
The broken inversion symmetry in the Janus configuration produces a significant and nearly isotropic Rashba spin splitting near the Γ-point, in addition to unique in-plane spin textures illustrating spin–momentum locking.

Our findings reveal that both pristine $AuBiO_3$ and Janus $Au_{0.5}Ag_{0.5}BiO_3$ monolayers serve as robust two-dimensional topological insulators. The improved bandgap and adjustable spin-orbit effects realised through Ag doping suggest that precise atomic substitution can effectively design new quantum materials. These results highlight the promise of $AuBiO_3$-based ilmenite oxides as flexible platforms for spintronic and quantum device applications.

Field of Condensed Matter:

Topological Materials

Materials and devices / 39

Bridging Memory and Intelligence at the Molecular Scale

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The exponential growth of data in the era of artificial intelligence and the Internet of Things demands new paradigms for storage and computation beyond conventional silicon. Here we report an organic, small-molecule–polymer memristor based on 2-mercapto-1-methylimidazole (MMI) blended with poly(4-vinylpyridine) (PVP) that unifies non-volatile memory and neuromorphic functionality in a single, scalable platform. The MMI:PVP heterolayer, confined between Ag or Cu electrodes in a metal–insulator–metal geometry, exhibits reproducible bipolar resistive switching with on/off ratios up to 6.9×10^3, retention exceeding 10^4 s, and endurance beyond 500 cycles. Depending on electrode composition and film thickness, the system transitions from digital to analog switching, enabling both binary data storage and gradual conductance modulation analogous to biological synapses. Pulse-driven potentiation, depression, and paired-pulse facilitation emulate short-term plasticity, while impedance spectroscopy and current–voltage scaling reveal a filamentary conduction mechanism governed by competing Ohmic, tunneling, and trap-assisted space-charge-limited currents. Density-functional calculations further elucidate redox-induced frontier-orbital reorganization that underpins the resistive states. This work establishes a lightweight, metal-ion-mediated molecular architecture for stable, low-power, and ambient-compatible organic memristors, bridging memory and computation at the molecular scale and advancing the vision of fully organic neuromorphic electronics.

Field of Condensed Matter:

Energy and Functional Materials

Amorphous / non-crystalline materials / **40**

Uncovering the role of structure for glasses with small-beam diffraction

Author: Amelia Liu[1]

[1] *Monash University*

Glasses pose many unique scientific and engineering problems. For crystals, the appearance of long-range periodic order is intimately linked to the solid phase. In contrast, glasses solidify from the melt with the disordered structure of the liquid. Crystals deform via the creation and propagation of dislocations that are defects in the order parameter field. For glasses, the structural transformations that mediate deformation, and cause brittle mechanical failure are not known. How can we understand the role structure plays in the nature and properties of glass?

Part of the problem is that unlike crystals, you cannot solve the structure of glasses uniquely with conventional, broad beam crystallography. A promising direction is to shrink your coherent beam down to the size of the correlated structures in a glass [1,2] and obtain "speckle" diffraction patterns. The information in these patterns is extremely rich and can be used to quantify local order in glasses [1], examine structural and dynamical heterogeneity [3] and understand strain localization and shear banding [3,4]. Scanning, small, coherent beam diffraction is a versatile experimental platform to link local structure in glasses to global behaviours.

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Authors acknowledge use of the Monash Centre for Electron Microscopy (ARC LE045416, LE200100132), the SAXS/WAXS beamline at the Australian Synchrotron and ARC support (FT180100594, DP250102966).

Field of Condensed Matter:

Noncrystalline materials and physics

Magnetism / **41**

2D van der Waals Magnets: From Fundamental Physics to Applications

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[1] *Seoul National University (SNU)*

The discovery of magnetism in atomically thin materials has opened an entirely new chapter in the study of low-dimensional quantum matter. Since the first reports of antiferromagnetic van der Waals magnets in 2016, followed by the discovery of ferromagnetic counterparts in 2017, the field has evolved into one of the most vibrant areas of condensed matter physics. In this talk, I will give a comprehensive overview of the key developments in the field of 2D vdW magnetism, drawing from my recent review.
I will begin with the historical and theoretical context, explaining why 2D magnetism was once thought to be impossible, and how recent materials have overcome these constraints. I will then

discuss the rapidly expanding family of van der Waals magnets, their underlying spin Hamiltonians, and experimental platforms for probing magnetic excitations, chirality, and phase transitions. The talk will also highlight surprising phenomena such as magnetic excitons, Floquet-engineered states, and light-induced metastable phases.
On the application side, I will describe how these materials are being integrated into spintronic architectures, with progress toward reconfigurable memory, spin filters, and ultrafast switching devices. I will conclude with an outlook on key open questions, emerging directions, and the future for this still-young but rapidly maturing field.
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Field of Condensed Matter:

Magnetism

Materials and devices / **42**

Polaron-Engineered Ultrasensitive X-ray Detectors in BiOCl Single Crystals

Author: SHUHUA YAO[1]

[1] *Nanjing university*

X-ray detectors are indispensable across medical diagnostics, security screening, space exploration, etc., yet their sensitivity and detection limit remain fundamentally constrained by the inherently physical compromises. Despite decades of optimization, persistent bottlenecks, including poor charge transport efficiency, rapid carrier recombination, environmental toxicity (e.g., CdTe/HgI2), and instability, have hindered the progress towards low-dose detection, which is essential for human safety and precision imaging. The manipulating electron-phonon interaction (EPI) and associated polaronic effects on carrier dynamics play a crucial role in achieving superior efficiency and sensitivity, however being largely overlooked. Here, the manipulation paradigm, by engineering the carrier transport from extrinsic to nearly intrinsic small-polaron, is successfully exemplified in layered BiOCl crystals. Under the nearly intrinsic small polaron transport configuration, we unveiled unprecedented detector metrics: record-high sensitivity (3.53 $mC \cdot Gyair^{-1} \cdot cm^{-2}$), ultralow detection limit (3.0 $nGyair \cdot s^{-1}$), charge collection efficiency with ultrahigh multiplication gain (12,698.77%), and stable operation (<33 pA dark current at 10 V). Optical spectroscopy and transport measurements confirm that these excellent properties stem from the small polarons in BiOCl, which exhibit two-order carrier lifetime (16.4 μs) longer than conventional semiconductors. The prototypical devices demonstrate exceptional X-ray imaging capabilities. It is anticipated that validation of small-polarn engineering in BiOCl to realize ultra-sensitive radiation detection as a universal paradigm surely promotes the fundamental design and development for new-generation detection materials.

Field of Condensed Matter:

Energy and Functional Materials

Nanoparticles / **43**

Behaviour of Gold Nanoparticles Under Compression

Author: Samuel Case[1]

Co-authors: Jodie Bradby [1]; Patrick Kluth [1]; Qianqian Shi [2]; Shankar Dutt [1]

[1] *Australian National University*

[2] *University of Newcastle*

Gold nanoparticles offer a promising route for probing stress and deformation at the nanoscale in diamond anvil cell (DAC) experiments. This project investigates how gold nanorods, nanobipyramids and related morphologies respond to compression, with a focus on assessing their potential as indicators of shear stress. We employ a multimodal characterisation approach combining in situ small-angle X-ray scattering (SAXS), scanning electron microscopy (SEM), Raman spectroscopy of the pressure medium, and synchrotron X-ray diffraction (XRD) measurements. SAXS provides sensitivity to particle shape and orientational behaviour, SEM captures post-compression morphology, Raman spectroscopy tracks hydrostaticity, and XRD allows correlation to crystallographic strain and defect development. Together, these complementary methods build a comprehensive picture of nanoparticle mechanics under pressure and evaluate the feasibility of using shape-anisotropic nanoparticles as nanoscale shear probes in high-pressure environments.

Field of Condensed Matter:

Noncrystalline materials and physics

Amorphous / non-crystalline materials / **46**

New developments for the application of polarised neutron scattering for magnetic and soft matter samples at ACNS

Author: Andrew Manning[None]

The spin polarisation of neutron beams can significantly enhance the information derived from scattering measurements for both magnetic and non-magnetic samples. At the Australian Centre for Neutron Scattering (ACNS), we are developing and using polarisation capabilities on several scattering instruments for the study of a variety of types of systems including altermagnets, high-temperature superconductors and liquid polymer solutions. This presentation will outline some recent developments with the instrumentation, experimental techniques and scientific outcomes related to these efforts. Current and future updates to the metastable exchange optical pumping polarisation station will be outlined, as well as some new beamline instrumentation options and upgrades to the polarisation capabilities intrinsic to several instruments. Furthermore, recent results such as studies of liquid matter dynamics in the quasi-elastic neutron scattering regime, magnon polarisation in an altermagnet, and the magnetic pair distribution function of a perovskite system will be discussed.

Field of Condensed Matter:

Noncrystalline materials and physics

Materials and devices / **47**

Uncovering Complex Phonon Interactions in Mg3Bi2-xSbx: Topology and Avoided Crossing

Author: LEI CHEN[1]

Co-authors: Kirrily Rule [2]; Weiyao Zhao [3]

[1] *University of Southern Queensland*
[2] *Australian Nuclear Science and Technology Organisation*
[3] *Monash University*

N-type Mg3(Sb,Bi)2 Zintl compounds are one of the most promising thermoelectric materials at near ambient conditions with excellent performance [1, 2]. In Mg3(Sb,Bi)2 compounds, one attracting property is the ultra-low lattice thermal conductivity (□□), which is believed to be dominated by the anharmonic lattice dynamics [3]. Another feature of Mg3(Sb,Bi)2 is topological phonon band structure [4], namely there is crossover area between the acoustic and optical phonon bands protected by crystal symmetry. However, the topological phonon bands have not been experimentally studied yet, nor their relationship with the ultra-low thermal conductivity. Herein, we present a systematic phonon study on Mg3(Sb, Bi)2 using both time-of-flight and triple-axis inelastic neutron scattering, supported by computational simulations based on density functional theory. We reveal a robust phonon band crossing between longitudinal acoustic and optical phonon branches along □ - M direction in the Mg3Bi1.5Sb0.5 single crystal, near which a significant broadening effect of the phonon modes has been located. Therefore, the enhanced phonon scattering process can be predicted due to the topological phonon band crossing, which will also contribute to the low □□ in this system. This finding provides an alternative avenue to predict, locate and engineer high performance thermoelectric materials with intrinsic ultra-low □□.

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Field of Condensed Matter:

Energy and Functional Materials

Experimental facilities in the Asia-Pacific / 48

Single crystal developments on Wombat, the high intensity neutron diffractometer at ANSTO

Author: Siobhan Tobin[1]

[1] *ANSTO*

The Wombat instrument is one of a few neutron diffraction instruments in the world to have a large position sensitive (effective area) detector, which has greatly supported the wide range of science applications and outcomes the instrument is able to undertake [1]. To date there have been limited single crystal studies undertaken on the Wombat instrument due to peak integration software being unavailable. Recently, we have liaised with the developers of the software INT3D [2] to overcome this. The work presented will showcase recent experiments on Wombat that have utilised this new analysis pipeline, as well as the Eulerian cradle with cryostat option. Coupled with this development in single crystal analysis, there is also work afoot to streamline crystallographic texture and diffuse scattering measurements on the instrument, which would also make full use of the detector capability.

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Field of Condensed Matter:

Magnetism

Magnetism / **50**

Topological hybridisation of plasmons with ferrimagnetic magnons

Authors: Cooper Finnigan[1]; Dmitry Efimkin[1]; Mehdi Kagarian[2]

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Polar transition metal dichalgenides (TMDs) host electronic states with strong Rashba spin orbit interactions, yielding two spin-split Fermi surfaces with opposite spin chirality. Electrons of each chirality have an electron spin constrained perpendicularly to the electron momentum, and as a result the collective plasmon excitations of polar TMDs present themselves as coupled charge- and spin density waves. Here we demonstrate that at the interface between a polar TMD and an insulating ferrimagnet, the plasmon excitations strongly hybridize with the ferrimagnetic magnon excitations. Due to the inequivalence of magnetic sublattice sites, ferrimagnetic magnons carry a magnetic dipole moment without any external magnetic field, and are thus spin-polarised, leading to strong exchange-mediated coupling between plasmons and magnons. Moreover, we show that the hybrid plasmon-magnon modes are topologically non-trivial due to the phase winding of the coupling between magnons and plasmons, which is inherited from the spin-momentum locking of the electronic states.

Field of Condensed Matter:

Magnetism

Condensed matter theory / **51**

Exact subtraction of electron self-interaction from the Kohn-Sham equations

Author: John Ingall[1]

Co-author: Alister Page [1]

[1] *The University of Newcastle, Australia*

The effective design of new materials for sustainable energy conversion can be facilitated by the accurate prediction of electronic properties with moderate computational complexity and cost. The self-interaction error (SIE) of Kohn-Sham density functional theory (KS-DFT) leads to a non-physical, non-linear dependence of an orbital's energy on its own fractional occupation [Dabo et al., Phys. Rev. B, 82:115121, 2010]. A generalized piecewise-linearity condition (GPWL) ensures an atomic orbital's eigenenergy is free of self-interaction. In this work, the effective potential of the Kohn-Sham equations is thereby constrained to be orbital-density dependent, with a total energy functional linear with respect to variation of its orbital densities. That is, the KS multiplicative effective potential $v_{\mathrm{s}}[n]$ for an orbital $\varphi_i[n]$ is constrained to a functional $v_{\mathrm{eff}}[n - n_i]$. The result complies with the Hohenberg-Kohn theorems. Fundamental band gaps of various semiconductor materials show an accuracy comparable to state-of-the-art many-body perturbation theory (MBPT). The result is an accurate, ab initio method with a computational cost comparable to the generalized gradient approximation (GGA) of KS-DFT.

Field of Condensed Matter:

Theory

Magnetism / **52**

Electromagnetic Responses in Antiferromagnets with Broken Time-Reversal Symmetry

Author: Rina Takagi[1]

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Antiferromagnets have long been regarded as magnetically compensated systems that lack the spontaneous electromagnetic responses characteristic of ferromagnets. However, recent advances in both experiment and theory have revealed that antiferromagnetic order can host a rich variety of electromagnetic phenomena when combined with symmetry breaking and complex spin textures. In this talk, we will present our recent studies to uncover emergent electromagnetic responses arising from antiferromagnetism with broken time-reversal symmetry.

In the first part, we will present our recent findings that rare-earth-based intermetallics with centrosymmetric tetragonal crystal structures can host nanoscale magnetic skyrmion lattices, exhibiting relatively large topological Hall effects. Our target material system features a layered crystal structure, where conducting layers alternate with magnetic rare-earth layers, resulting in strong coupling between conduction electrons and localized moments. Due to their centrosymmetric crystal structures, itinerant-electron-mediated magnetic interactions are expected to play a crucial role in the formation of nanoscale skyrmions. GdRu2Si2 hosts a square skyrmion lattice, while GdRu2Ge2 and EuAl4 exhibit square and rhombic lattices of skyrmions with multiple-step topological magnetic phase transitions. These features suggest that the symmetry of the skyrmion lattice is sensitive to the electronic structure and can be controlled through chemical substitution and external stimuli.

In the second part, we present our experimental observation of a spontaneous Hall effect in the collinear antiferromagnet FeS at room temperature. FeS hosts antiferromagnetically ordered Fe moments together with a staggered arrangement of non-magnetic S ions, giving rise to an altermagnetic electronic structure. Our analysis indicates that the spontaneous Hall effect originates from a momentum-dependent fictitious magnetic field intrinsic to the antiferromagnetic order lacking time-reversal symmetry.

Together, these results demonstrate that antiferromagnets can host a wide variety of unconventional electromagnetic responses and may lead to functionalities beyond the traditional ferromagnetic paradigm.

Field of Condensed Matter:

Magnetism

Magnetism / **53**

A general spin Hamiltonian for Rare Earth Orthochromites RCrO3

Author: Shinichiro Yano[1]

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The perovskite ABO_3 is a significant class of materials with properties, such as superconductivity, ferroelectricity, charge ordering, colossal magnetoresistance [1]. By substituting the crystallographic A- or B-site, the material can be tuned to increase potential for applications. Our focus is so-called orthochromites RCrO3 (R = rare earth, Sc, and Y). The RCrO3 has received much interest as an electrode material [2], an interconnector for solid-state fuel cells [3], and a magnetocaloric effect for

refrigeration [4]. However, there is little understanding because of availability of large single crystal samples [6]. It is important to understand RCrO3 together with the other outstanding perovskites RTiO3, RVO3, RMnO3, RFeO3 (S = 1/2, 1, 2, and 5/2), and so on [7].
In this presentation, I will present a series of inelastic neutron scattering experiments of orthochromites, such as, LaCrO3 (4.0 g), ErCrO3 (6.3 g) and HoCrO3 (3.5 g) and so on. We have performed a series of neutron scattering experiments on 4SEASONS, HRC at J-PARC and Wombat, Taipan, Emu, Sika at ANSTO. To describe the magnetic excitations, I am trying to find a general spin Hamiltonian consists of exchange interactions between Cr3+, Dzyaloshinskii-Moriya (DM) interactions, single ion anisotropic, exchange interactions between Cr3+ -R3+, crystal field excitations, hyperfine field excitations from R3+, and so on. I will describe the general overview of magnetic excitations from μeV to 100 meV in RCrO3

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Field of Condensed Matter:

Magnetism

Materials and devices / 54

Rare-Earth-Driven Noncollinear Magnetism in Magnetite: From Site Selectivity to Tuneable Magnetic and Thermoelectric Properties

Author: M. Hussein N. Assadi[1]

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We investigated site-selective Eu^{3+} substitution in Fe_3O_4 thin films to engineer noncollinear magnetism and enhance saturation magnetisation [1]. Our experiment was guided by KKR-CPA density functional calculations with self-interaction correction and spin-orbit coupling, which predicted that, at low Eu content (~ 0.05 at$\%$), tetrahedral site doping was more stable. We confirmed site occupancy via electrical resistivity measurements and valence-band spectroscopy, which differentiate between octahedral and tetrahedral substitution. Accordingly, tetrahedral Eu substitution preserves magnetite's half-metallicity with Eu 4f states emerging in the majority spin channel while minimally perturbing Fe 3d states near the Fermi level.

Furthermore, we observed a substantial increase in M_S to $\sim 4.4\ \mu_B$/f.u. for tetrahedral substitution, exceeding pristine $\sim 3.8{-}4.0\ \mu_B$/f.u. In contrast, octahedral substitution reduces M_S. Using XAS & XMCD, we determined that Eu^{3+} contributes a positive orbital magnetic moment with strong in-plane anisotropy, and its moment aligns parallel to octahedral Fe but antiparallel to tetrahedral Fe, reducing ferrimagnetic cancellation and boosting net magnetisation. The resulting magnetic structure deviates from Néel's collinear model due to Eu-induced noncollinearity. Our findings establish site-selective rare-earth substitution as a practical strategy to design high-M_S, anisotropic ferrimagnetic spinels by 4f doping.

Our extended work shows that rare-earth doping in magnetite can induce site-selective, spin-orbit-driven noncollinear magnetism, which in turn can increase saturation magnetisation [2], adjust the Curie temperature [3], and substantially enhance thermoelectric performance by lowering thermal conductivity [4]. This ability to fine-tune magnetite's magnetic behaviour is valuable for applications

such as self-regulated magnetic hyperthermia, energy conversion, and magnetically recoverable catalysts, thereby extending the utility of this common oxide to biomedical heating, tissue identification, and medical sensing.

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Field of Condensed Matter:

Magnetism

Condensed matter theory / **55**

Interplay of magnetic textures with spin-orbit coupled substrates

Authors: Eric Mascot[1]; Oleg Tretiakov[2]; Stephan Rachel[3]; Zachary Llewellyn[3]

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Skyrmions, first proposed as a model for nucleons by Tony Skyrme in 1961 [1] , have seen recent interest in past decades as a model for topologically protected vortex-like magnetic spin textures with extensive applications in spintronics [2] and topological quantum computing [3]. This talk will be covering recent work [4] theoretically investigating thin-film skyrmion systems layered on substrates possessing spin-orbit coupling (SOC) and the connection between this substrate SOC and the induced SOC from the skyrmion itself. Our key finding is that substrate SOC and the SOC contributions induced by the magnetic texture, generally, do not simply add, as intuitively expected but have a more complex relationship. We begin with a discussion about spintronic gauge theory and the induced SOC and magnetic fields that appear from the interplay between skyrmion textures and substrate SOC. Following this we provide a theoretical marker for observing the SOC arising from substrate-skyrmion interplay using direction-dependent spin-projected currents. Finally, we will conclude with a mesoscopic study on the symmetries present between various skyrmion types in the presence of Rashba and Dresselhaus SOC.

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Field of Condensed Matter:

Magnetism

Magnetoelastic coupling and magnetic phase transition in ThMn12-type TbFeNb

Authors: S.J. Campbell[1]; Wayne Hutchison[2]

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The structural and magnetic properties of TbFe11.35Nb0.65 (space group I4/mmm) have been investigated systematically via high resolution synchrotron x-ray diffraction and magnetic measurements. The temperature dependence of the lattice parameters exhibits abnormal phenomena around the spin reorientation temperature Tsr = 415(5) K and Curie temperature TC = 583(5) K. The variations of Wigner-Seitz cell (WSC) volume, the bond lengths between each site (2a, 8i, 8j and 8f) and the adjacent Fe atoms as well as the atomic coordinates with changing temperature demonstrate the existence of magnetoelastic coupling. Below TC, there exists large spontaneous magnetostriction in both the a and c directions. The spontaneous volume magnetostriction ωs at 100 K is derived to be ωs = -8.19×10-2.

Detailed analyses of the critical magnetic behaviour around TC show that the critical exponents β, γ and δ are consistent with the values of the mean-field model. Spectral fitting of the Mössbauer spectrum indicates that the Nb atoms exclusively occupy the 8i site with the hyperfine interaction parameters determined for the 8i, 8j and 8f sites.

We acknowledge and appreciate support from the Australian Research Council, the Australia Synchrotron and ANSTO.

Field of Condensed Matter:

Magnetism

Magnetism / **59**

Revealing Skyrmion Behaviour Through Simultaneous Doping in Cu_2OSeO_3

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Magnetic skyrmions are topologically protected spin structures that can be manipulated by various external stimuli with minimal energy input, making them attractive for future spintronic applications [1]. Skyrmion hosting materials have been proposed as solutions for many current global issues, especially around energy consumption and usage, with the potential for skyrmion hosts to provide more energy-efficient memory devices with quicker storage and retrieval of information [2,3]. Cu₂OSeO₃ was the first insulating multiferroic material observed to host magnetic skyrmions under specific conditions [4]. It possesses a magnetic structure with both ferromagnetic and antiferromagnetic superexchange interactions and has a 3-up 1-down ferrimagnetic arrangement of Cu²⁺ ions [5]. The competition between Heisenberg exchange and Dzyaloshinskii–Moriya interactions induces a gradual canting of spins, which under specific conditions stabilises skyrmion textures: $H = -\sum_{ij} J_{ij} S_i \cdot S_j + \sum_{ij} D_{ij} \cdot [(S_i) \times (S_j)] - h_0 m$ [4]. Previous research has focused on doping either the magnetic (Cu²⁺) or non-magnetic (Se⁴⁺) sites individually, observing changes to the skyrmion formation conditions through X-ray, neutron and magnetisation techniques [6–8]. Upon doping, the magnetisation and direction of the competing interactions are altered. The current project aims to investigate the effects of doping both metal sites simultaneously, allowing for a further understanding of the formation of skyrmions.

In this work, (Cu_{1-x}Zn_x)₂O(Se_{1-y}Te_y)O₃ $[0 \leq x \leq 0.2]$ $[0 \leq y \leq 0.2]$ was synthesised with the lattice expanding upon positive chemical pressure. The strong Cu2-Cu2 ferromagnetic interactions decrease in length while the weak and strong Cu1-Cu2 antiferromagnetic and the weak Cu2-Cu2 ferromagnetic interactions increase, resulting in the Cu-Cu interactions elongating overall. Magnetisation studies show a change in the magnetic transition temperatures upon doping, which varies to both the undoped and single-doped samples. Additionally, a drop in the magnetic saturation was observed, which differs from the single-doped samples, along with differences in the observed magnetic phases using small-angle neutron scattering under specific conditions.

Field of Condensed Matter:

Magnetism

Spectroscopies 1 / 60

Li-ion Dynamics in Solid Electrolytes: An Integrated Neutron-based techniques and Terahertz Time-Domain Spectroscopy Study

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All-solid-state batteries (ASSBs) hold significant commercial promise, driven by their inherent potential to deliver exceptional energy density, power density, and safety. While factors such as rate capability, interfacial stability, and extended cycle life hinder the development of ASSBs, which are critically dependent upon ionic conductivity enhancements within solid-state electrolytes (SSEs). Among SSE families, Li7La3Zr2O12 (LLZO) demonstrates exceptional commercialization potential due to its intrinsic compatibility with lithium metal and outstanding thermal stability under ambient conditions. However, in Li-ion SSEs, the intricate Li+ migration dynamics remain inadequately understood, critically constraining rational materials design.
In this study, Nb mono-doped and Ta/Nb equimolar co-doped LLZO samples (Li6.4La3Nb0.6Zr1.4O12 and Li6.4La3Ta0.3Nb0.3Zr1.4O12, respectively) were fabricated via spark plasma sintering (SPS). Implementing neutron powder diffraction (NPD) at ANSTO, we have obtained Li-ion-centric crystallographic information, which is more reliable than conventional lab-based X-ray powder diffraction. Inelastic neutron scattering (INS) revealed the energy distribution, population, and Q-dependence of Li-centered vibrational modes, as well as the momentum-integrated Li-dominated phonon density

of states (DOS) that controls the attempt frequency and many-body phonon-ion coupling, which can only be isolated from the heavy La-O/Zr-O framework with neutron-based probes.
To reveal complementary microscopic mechanisms and to probe Li+ ions'transient pre-hopping behaviors, we implemented in situ THz time-domain spectroscopy (THz-TDS) to drive ultrafast on-site Li+ ions vibrating at their intrinsic oscillation frequencies (~1012 -1013 s-1). Fourier transforming spatiotemporal resolved spectra, , we yielded frequency spectra, then computed the THz conductivity that is dominated by localized vibrational modes coupled to polar lattice phonons.
Overall, this study serves as a proof of concept for utilizing Neutron-based and THz-TDS to probe ion dynamics in ionic conductors. Also, we have shown the scientific workflow to delve the mechanistic insights with these techniques.

Field of Condensed Matter:

Energy and Functional Materials

Transition metal dichalcogenides / **61**

Strong spin-orbit interaction in van der Waals α-In2Se3

Authors: Peng Zhang[1]; Dongchen Qi[1]

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α-In_2Se_3 has attracted enormous research attention due to its intrinsic ferroelectricity since 2017. However, the transport properties of α-In_2Se_3 are rarely reported due to relatively low mobility. In this paper, we report systematic experimental studies on magnetoresistance measurement of α-In_2Se_3 thin flakes. We observed strong spin-orbit interaction probed by weak anti-localization (WAL). We found giant variation of conductance exceeding 100 G_0 ($G_0 = e^2/\pi h$) at low magnetic field B = 0.1 T, where the magnetoconductance exhibits layer-dependency. The WAL magnetoresistance and phase-coherence agree well with the Hikami, Larkin, and Nagaoka (HLN) theory. These results demonstrate α-In_2Se_3 as a potential material for high performance spintronic applications.

Field of Condensed Matter:

Quantum Materials

Materials and devices / **62**

Engineering Diamond Surfaces for Quantum Diamondtronics

Author: Dongchen Qi[1]

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Despite being a bona-fide bulk insulator, diamond develops an intriguing two-dimensional (2D) p-type surface conductivity when its surface is terminated by hydrogen and exposed to appropriate surface adsorbate layer such as atmospheric water as a result of the surface transfer doping process. Consequently, the surface of diamond presents a versatile platform for exploiting some of the extraordinary physical and chemical properties of diamond, leading to applications such as chemical/biological sensing and the development of high-power and high-frequency field effect transistors (FETs).

In this talk, I will describe our recent work on the surface transfer doping of diamond by transition metal oxides (TMOs). Specifically, I will show that by interfacing diamond with MoO_3 or V_2O_5 a 2D hole conducting layer with metallic transport behaviours arises on diamond. The 2D hole layer affords a surprisingly large spin-orbit interaction giving rise to exotic quantum coherent spin transport properties as revealed by low-temperature magnetotransport. The spin transport can be further tuned by an external electric field in a metal-oxide-semiconductor FETs (MOSFETs) architecture. I will also introduce our recent work on the formation of transferrable dielectric layers on diamond through van der Waals integration to enable high-performance p-channel diamond surface electronics. Lastly, the hydrogen-terminated surface of diamond affords an ultralow surface energy that allows the pick-and-place transfer of arbitrary metal electrode arrays for van der Waals device fabrication. This novel diamond-assisted electrode transfer technique enables us to realise van der Waals integration of wafer-scale prefabricated electrode arrays onto 2D materials, enabling scalable 2D electronics and optoelectronics.

Field of Condensed Matter:

Quantum Materials

Spectroscopies 1 / 63

Ultrafast Magnetisation Dynamics Driven by Terahertz Light Fields via Spin Hall and Rashba–Edelstein Effects

Author: Sergey Kovalev[1]

Co-authors: Anneke Reinold [1]; Igor Ilyakov [2]; Ruslan Salikhov [2]; Steffen Kober [1]; Zhe Wang [1]

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Ultrafast control of magnetisation states in magnetically ordered systems represents a key technological challenge for developing memory devices operating on picosecond timescales. This challenge has stimulated extensive research into ultrafast magnetisation dynamics, spin transport, and magnetoresistance phenomena across a wide range of conventional and emerging magnetic materials. To achieve coherent manipulation with light fields, terahertz (THz) radiation has been proposed as a driver due to its picosecond field oscillations and thus strong ponderomotive potential. We have demonstrated THz-field-driven generation of spin currents via the spin Hall effect and the ultrafast spin Seebeck effect. These mechanisms enabled THz spin–orbit torque-driven high-energy magnon excitation and spintronic frequency multiplication. However, the coupling between light-field-driven spin currents and magnetoresistance effects at optical frequencies remains largely unexplored.
Unidirectional spin Hall magnetoresistance (USMR) provides a simple two-terminal geometry for electrical detection of magnetisation states in magnetic heterostructures. Conventional USMR has been observed under direct current at low frequencies (kHz range), but its operation at light frequencies has not yet been investigated. Using nonlinear THz spectroscopy, we report an ultrafast version of the USMR effect in magnetic heterostructures, manifested through THz second-harmonic generation detected in a far-field configuration. By analysing the in-plane angular dependence between THz polarisation and sample's magnetisation orientation, we disentangle the USMR contribution from thermally driven spintronic frequency multiplication processes. Moreover, at interfaces exhibiting pronounced inversion symmetry breaking, Rashba–Edelstein effects participate in the magnetoresistance dynamics, offering additional tunability toward 2D magnetic heterostructures.
Our results enable non-destructive studies of light-field-driven spin-dependent scattering dynamics in magnetic heterostructures based on heavy metals or Rashba-split systems, providing new insights into ultrafast magnetism and advancing THz spintronics.

Field of Condensed Matter:

Magnetism

Thin films / **64**

Three-dimensional flat band in ultra-thin Kagome metal Mn3Sn film

Authors: James Blyth[1]; Mengting Zhao[1]

Co-authors: Anton Tadich [2]; Mark T. Edmonds [1]; Michael S. Fuhrer [1]

[1] *Monash University*

[2] *Australian Synchrotron*

Flat bands with narrow energy dispersion can give rise to strongly correlated electronic and topological phases, especially when located at the Fermi level. Whilst flat bands have been experimentally realized in two-dimensional (2D) twisted van der Waals heterostructures, they are highly sensitive to twist angle, necessitating complex fabrication techniques. Geometrically frustrated kagome lattices have emerged as an attractive alternative platform as they can natively host flat bands which have been observed experimentally in quasi-2D bulk-crystal kagome metals. An outstanding experimental question is whether flat bands can be realized in ultra-thin metals, with opportunities for stronger electron-electron interactions through tuning of the surrounding dielectric environment. Here we use angle-resolved photoelectron spectroscopy, scanning tunnelling microscopy and band structure calculations to show that ultra-thin films of the kagome metal Mn3Sn host a robust dispersionless flat band with a bandwidth of 50 meV. Furthermore, we demonstrate chemical tuning of the flat band to near the Fermi level via manganese defect engineering. The realization of tunable kagome-derived flat bands in an ultra-thin kagome metal, represents a promising platform to study strongly correlated and topological phenomena, with applications in quantum computing, spintronics and low-energy electronics.

Field of Condensed Matter:

Magnetism

Experimental facilities in the Asia-Pacific / **66**

Introducing NANO: Australia's New Hard X-ray Nanoprobe Beamline

Author: Evan Constable[1]

Co-authors: Cameron M. Kewish [1]; Martin D. de Jonge [1]

[1] *ANSTO - Australian Synchrotron*

The BRIGHT upgrade to the Australian Synchrotron is delivering eight new beamlines, expanding the capabilities of our synchrotron facility by enabling cutting-edge science across multiple disciplines. Among these, the Nanoprobe beamline (NANO) is one of the most technically ambitious, designed to deliver hard X-ray fluorescence and diffraction mapping at spatial resolutions down to 60 nm, with super-resolution phase-contrast imaging expected to extend below 15 nm using ptychography.

Achieving this requires many special considerations for an instrument spanning over 100 m, with the endstation housed in a dedicated satellite building. Key optical components include a double multilayer monochromator for high-flux, energy-selective photon delivery, a secondary source aperture for coherence control, and a pair of Kirkpatrick–Baez mirrors for primary focusing. In this context, mechanical and thermal stability are critical, necessitating innovative engineering solutions to meet the stringent requirements of nanometric precision.

From day one, the beamline will support elemental mapping (Si–U) via fluorescence, ptychography, differential-phase contrast imaging, and multimodal tomography, as well as providing a platform for development of nanobeam mapping techniques based on coherent small-angle scattering and diffraction. A future upgrade will introduce spectroscopy via the addition of a double-crystal monochromator. The true power of NANO lies in its ability to integrate these complementary techniques into a single platform, enabling nanoscale sampling with broader real-space and reciprocal-space context.

Thus, NANO brings the Australian Synchrotron into the nanoscale, offering exciting new opportunities for condensed matter physics studies. Potential use cases include nanoscale analysis of quantum materials, layered heterostructures, and strain fields in functional devices. We invite the condensed matter community to engage with us in shaping the scientific direction of the beamline through collaboration, capability development and novel experiment proposals. With first light expected mid-2026 and user operations commencing later that year, we look forward to welcoming you to NANO.

Field of Condensed Matter:

Energy and Functional Materials

Topological materials / **67**

On-surface synthesis of metal-coordinated and covalently-bonded monolayer networks based on 1,3,5-tribromobenzene

Author: Brody Tallon[1]

Co-authors: Agustin Schiffrin [2]; Jennifer Macleod [1]; Josh Lipton-Duffin [1]; Kathleen Mullen [1]

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Metal-organic frameworks (MOFs) and covalent organic frameworks (COFs) provide a highly tuneable route for synthesising 2D materials with desirable electronic properties. A key focus of recent research has been dedicated to synthesising two-dimensional honeycomb and kagome MOF/COFs on surfaces with atomic precision. These lattice structures have attracted significant interest due to the intrinsic role that strong electron correlations and non-trivial band topology can play in their electronic properties, offering a versatile platform for exploring exotic quantum phases in 2D materials.

We report preliminary scanning tunnelling microscopy (STM) results investigating the on-surface synthesis and structure of honeycomb/kagome networks derived from 1,3,5-tribromobenzene on Ag(111) and Au(111) substrates under ultra-high vacuum (UHV) conditions. We present an exploration of the parameter space, with a particular focus on how annealing temperature and the choice of metal centre, facilitated through deposition of the selected metal species, affect the structures produced. These preliminary results demonstrate the temperature-dependent reaction pathways for forming honeycomb/kagome metal-coordinated and covalently-bonded monolayers from a brominated precursor on metallic substrates, providing a platform for investigating their unique electronic properties.

Field of Condensed Matter:

Quantum Materials

Spectroscopies 1 / **68**

Raman signature of cation vacancies in rare-earth nitrides

Author: Martin Markwitz[1]

[1] *Victoria University of Wellington*

The rare-earth mononitrides (LnN, Ln a lanthanide) form a mutually epitaxy-compatible series of ferromagnetic semiconductors with promise for mixed superconductor-spintronics.[1] Their varying occupation of 4f states precipitate enormously varied and useful magnetic properties, the topic of intense recent investigation toward those applications.[2,3] Their electrical properties can be controlled independently to their magnetic properties by tuning the deposition conditions to incorporate nitrogen vacancies. The usage of ionized or molecular nitrogen, which catalytically reacts at the surface at ambient temperatures provides capacity for nitrogen-vacancy rich LnN to be formed, and therefore very conductive LnN films to be made. [4,5] Here Raman spectroscopy on the LnN and the identification of Ln vacancies are discussed via the identification of a high-frequency cation-centered symmetric N breathing mode.

This research compares the Raman peak mode frequencies and breathing modes about cation vacancies computed using density functional theory (DFT) for a variety of LnN: LaN, GdN, ErN, and LuN. We find excellent agreement with the measured LnN cation vacancy breathing mode frequencies when using a combined Hubbard U parameter correction approach applied to the 4f and 2p states of Ln and N, respectively. In conclusion, the capacity to incorporate and identify the presence of cation vacancies in a family of compounds otherwise restricted to n-type transport opens the door for p-type material discovery in the rare-earth mononitrides.

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Field of Condensed Matter:

Energy and Functional Materials

Topological materials / 69

Weyl magneto-plasma waves in magnetic Weyl semimetals

Author: Dmitry Efimkin[1]

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The recent surge of interest in Weyl materials is driven largely by the rich variety of fundamental topological phenomena they exhibit, including the chiral anomaly, topological surface states, and unconventional transport regimes. These discoveries have inspired the search for Weyl excitations not only in electronic systems but also in magnetic, photonic, and acoustic platforms. In particular, Weyl-like features have been predicted and observed in magnetoplasma oscillations of magnetized electron gases.

In this talk, I will argue that Weyl magnetoplasma oscillations also arise naturally in magnetic Weyl semimetals as a consequence of the topological anomalous Hall response. These excitations originate from the hybridization of circularly polarized electromagnetic waves with linearly polarized plasmon modes. Using both analytical and numerical approaches, we demonstrate that the resulting nontrivial topology gives rise to exotic Fermi–arc–like interface modes localized at magnetic domain walls separating regions with the opposite magnetization.

1. D.K. Efimkin and S. Syzranov - **Weyl excitations via helicon-phonon mixing in conducting materials -** Phys. Rev. B 108, L161411 (2023)
2. Y. Wang, O. V. Kotov, and D. K. Efimkin - **Weyl magneto-plasma waves in magnetic Weyl semimetals** - In preparation

Field of Condensed Matter:

Topological Materials

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Topological magnons and phonons in Kitaev magnets

Author: Kwang-Yong Choi[1]

[1] *Sungkyunkwan University*

The celerated Kitaev spin model offers a paradigmatic platform for exploring distinct topological phases tunable by magnetic fields, anisotropies, and the sign of Kitaev exchange interactions. Under a magnetic field, the Majorana spinon bands acquire nontrivial topological invariants, driving a transition from a trivial Z_2 spin liquid to a Chern Majorana insulator with chiral edge modes and quantized thermal Hall conductance. In the field-polarized regime, magnons also develop nontrivial Chern numbers across a broad field range.
In this presentation, we investigate the evolution of low-energy quasiparticle excitations in the Kitaev candidate material α-$RuCl_3$ across magnetic fields up to 29 T, revealing how sharp magnon modes emerge from the fractionalized Majorana continuum. By combining Raman circular dichroism with in-plane angular measurements, we uncover the sixfold symmetry of topological magnons and two-magnon excitations reflected in their Chern number changes, along with emergent topological phonons arising from magnon–phonon hybridization. These observations provide fresh insights into the topological structures of bosonic excitations in real Kitaev materials.

Field of Condensed Matter:

Magnetism

72

Magnetic phase evolution and Griffiths Phase behavior in $PrMn_xCr_{1-x}O_3$ $(0 \leq x \leq 1)$

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We investigated the magnetic behavior of $PrMn_xCr_{1-x}O_3$ ($0 \leq x \leq 1$) using neutron powder diffraction and DC magnetization. All samples show a Griffiths phase (GP) above the main magnetic ordering temperature (T_N/T_C), indicating short-range ferromagnetic (FM) clusters within a paramagnetic matrix. For $x = 0.25 - 0.5$, the GP appears in two steps, suggesting two classes of FM clusters with different energy scales. With increasing Mn content, the GP becomes stronger, as shown by larger Griffiths exponents and broader singularity regions, consistent with larger and more stable FM clusters. The ordering temperature decreases from 237 K at $x = 0$ to 75 K at $x = 0.6$, then remains nearly constant ($76 - 87$ K) at higher Mn levels. This reflects competition between antiferromagnetic (AFM) and FM interactions. Below T_N/T_C, samples with $x = 0 - 0.6$ adopt the Γ_5 (G_z, F_x) magnetic structure, dominated by G-type AFM order with weak FM canting at $x = 0$. Increasing Mn weakens the AFM G_z component and strengthens the FM F_x component, which becomes dominant at $x = 0.6$. Upon further cooling, Pr^{3+} moments polarize, forming the Γ_5 (G_z, F_x; F_x^{Pr}) phase for $x = 0.2 - 0.6$. At ∼20 K, these compositions transition to Γ_5 (G_z, C_y, F_x; F_x^{Pr}). For $x = 0.75 - 0.8$, magnetic ordering at T_C follows the Γ_7 (F_y; F_y^{Pr}) structure. Around 60 K, a mixed Γ_7 (F_y; F_y^{Pr}) + Γ_3 (A_y) phase emerges. Cooling to ∼30 K introduces an F_z component within Γ_3, producing a mixed Γ_7 (F_y; F_y^{Pr}) + Γ_3 (A_y, F_z) structure. For $x = 1$ ($PrMnO_3$), the system stabilizes in the Γ_3 (A_y) phase without further transitions.

Field of Condensed Matter:

Magnetism

Magnetism / **73**

Exploring Magnetic Phase Transitions of Helimagnets Using Neutron and Resonant Elastic X-ray Scattering

Authors: Yu-Hui Liang[1]; Chun-Hao Lai[2]; Chin-Wei Wang[3]; Shinichiro Yano[3]; Daisuke Okuyama[4]; Taku Sato[5]; Shih-Chang Weng[3]; Yen-Chung Lai[3]; Wei-Tin Chen[6]; Kirrily Rule[7]; Chao-Hung Du[2]

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Investigating the phase transitions of magnetic materials offers valuable insights into their fundamental physical mechanisms, thereby broadening the scope of their potential applications. While neutron scattering techniques are commonly employed by researchers for such studies, resonant elastic scattering using synchrotron radiation also proves highly effective in this field. The double-perovskite YBaCuFeO5 exhibits two magnetic phase transitions at *T*_{N1} ~ 455 K and *T*_{N2} ~ 175 K, respectively. Below *T*_{N2}, the magnetic structure transforms from commensurate into a spiral magnetic structure with a propagation vector of (h/2 k/2 l/2+δ), incommensurability δ depending on temperature. Using elastic neutron scattering and resonant elastic x-ray scattering, this spiral structure was observed to consist of two spiral spin orderings originating from Fe³⁺ and Cu²⁺, respectively, i.e., forming a double-spiral spin ordering. In addition, under an applied magnetic field, neutron scattering measurements reveal more intricate magnetic structures, accompanied by pronounced thermal and magnetic hysteresis effects. We have successfully constructed the H-T phase diagram by employing high-quality single-crystal samples, offering deeper insights into the material's magnetic behavior.

Field of Condensed Matter:

Magnetism

Materials and devices / 74

Emergent interlayer coupling in near-quasicrystalline twisted bilayer graphene

Author: Kuo-En Chang[1]

Co-authors: Aitor Garcia-Ruiz [1]; Ta-Lei Chou [2]; Yen-Ting Liu [1]; Sheng-Chin Ho [1]; Yu-Chiang Hsieh [1]; Ching-Hua Kao [3]; Li-Ying Chen [3]; Chiu-Hua Huang [1]; Kenji Watanabe [4]; Takashi Taniguchi [5]; Ming-Wen Chu [2]; Ming-Hao Liu [1]; Tse-Ming Chen [3]

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Twistronics has revealed a wide variety of emergent quantum phenomena [1, 2], but predominantly at small twist angle where interlayer hybridization is strong, whereas large-angle systems are conventionally regarded as electronically decoupled. At 30°, the bilayer forms a quasicrystalline configuration, and recent spectroscopy has reported unexpectedly strong interlayer hybrization at high energies, far from the Fermi level [3, 4]. This has led to increasing interest in bringing these high-energy coupling effects into the low-energy regime, either by twisting trilayer graphene to generate two moiré sets [5] or by employing materials that have flatter dispersion such as WSe2 [6].

Here, we investigate twisted bilayer graphene at large angles, focusing on the crossover between the 27.8° commensurate moiré superlattice and the 30° quasicrystal. The structural evolution between these two regimes is uncovered using transmission electron microscopy (TEM). Low-temperature transport measurements combined with theoretical modelling further demonstrate the emergence of unexpectedly strong low-energy interlayer coupling driven by Umklapp scattering, accompanied by unconventional electronic features. These findings challenge the conventional view that large-angle twisted bilayers are electronically decoupled and establish the near-quasicrystal regime as a viable platform for emergent phenomena.

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Field of Condensed Matter:

Quantum Materials

Magnetism / 75

Rare earth nitrides - ferromagnetic semiconductors for energy-efficient superconducting and quantum electronics

Author: Simon Granville[1]

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Combining the rare earth (lanthanide) elements with nitrogen results in the rare-earth nitrides, semiconducting materials with strong magnetic moments that order cooperatively at cryogenic temperatures. The resulting materials have both highly-tuneable magnetism and conductivity that can be controlled over orders of magnitude –a near-unique combination with multiple applications for energy-efficient cryogenic and quantum electronics [1].
In this presentation I will showcase some of the most intriguing and technologically relevant results from our 20 years of research on the rare-earth nitrides as thin films, including (nearly) zero moment ferromagnetic states [2], superconductivity [3] and large unquenched orbital magnetic moments [4]. These and other characteristics make the rare-earth nitrides potential solutions to ongoing challenges in developing energy-efficient cryogenic electronics, including as control electronics for quantum computing [5]. I will also show results from our recent work to develop the rare-earth nitrides into prototype cryogenic memories and superconducting circuit elements.

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Field of Condensed Matter:

Magnetism

Thin films / **76**

Light-Induced Structural and Optical Changes in Yb+3 doped in CsPbI2Br perovskite thin films

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In this work, we synthesised CsPb0.95Yb0.05I2Br perovskite thin films using a precursor solution-based technique. The perovskite solution was deposited onto a glass substrate via spin-coating. X-ray diffraction (XRD) analysis confirmed the successful formation of an orthorhombic single-phase structure with the space group Pbnm (No.57) via Rietveld refinement using Fullprof. Furthermore, the structural changes of the films under light exposure were explored using XRD, UV-Vis spectroscopy and photoluminescence (PL) spectroscopy. The XRD revealed a transition from an orthorhombic single phase to a double-phase structure characterised by space groups Pbnm and Pnma under light exposure. UV-Vis spectroscopy showed that the optical band gap decreased from an initial 1.89 eV to 1.76 eV after 2 hours of light exposure. Remarkably, when the sample was returned

to, and kept in the dark for 5 days, the band gap returned to 1.88 eV. PL measurements indicated a peak around 640 nm, which shifted with light exposure. After 2 hours of exposure to 430 nm LED light, the PL peak signal exhibited full recovery.

Field of Condensed Matter:

Energy and Functional Materials

Spectroscopies 1 / **77**

Phase-sensitive Surface Second-harmonic Generation of Topological Dirac Semimetal

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Topological semimetals are a new class of quantum materials characterized by symmetry-protected, nontrivial band crossings near the Fermi energy. These systems have attracted wide interest for their ability to host exotic quantum-transport and electromagnetic phenomena. Although bulk topological semimetals have demonstrated enhanced optical nonlinearities with promise for next-generation optoelectronic applications, intrinsic symmetry constraints often limit the scope of their nonlinear response. In contrast, the topological surface states (TSSs) of these materials have been predicted to support unconventional nonlinear optical signatures under relaxed symmetry conditions. However, surface nonlinear optics of topological materials has remained elusive, and whether it can be enhanced through TSSs is still unclear. In this work, we address this challenge by performing heterodyne-detected second harmonic generation (HD-SHG) spectroscopic study on a prototype Dirac semimetal PdTe₂. We find its reflected SHG to follow *C_{3v}* surface symmetry with a time-varying intensity governed by oxidation kinetics of the material after its surface cleavage, confirming the surface-derived origin of SHG. The complex anisotropic surface nonlinear optical susceptibility tensor χ⁽²⁾ for the pristine surface is fully characterized by heterodyne interferometry, unveiling a hidden giant response along the axis of rotational invariance (|χ⁽²⁾_{*zzz*}|=14±4 nm²/V, corresponding to an effective bulk susceptibility of 14±4 nm/V), where the protected Dirac cones are formed through band inversion. Surface- and orbital-projected band calculations further reveal the correlation of this unusual property to the nontrivial TSSs. Our results highlight the topological interfaces as a promising platform for achieving strong nonlinear optical responses under relaxed symmetry constraints and demonstrate HD-SHG as a powerful *in situ* probe of surface chemistry in topological systems.

Field of Condensed Matter:

Topological Materials

Materials and devices / **78**

Reaction Time Dependent Evolution of Graphene-hBN Lateral Heterostructures via Direct Chemical Conversion

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Graphene exhibits excellent carrier mobility and electrical conductivity. However, with its zero-bandgap nature, its applications in nanoelectronics which require on/off switching capabilities are limited. Introducing a bandgap while maintaining graphene's electronic properties is achieved by forming heterostructures with hexagonal boron nitride (hBN). Having a wide bandgap (˜6 eV) and close lattice matching with graphene (lattice mismatch ˜1.7%), hBN enables the formation of high-quality lateral heterostructures [1]. Conventional chemical vapor deposition methods on metallic substrates require subsequent transfer steps that introduce mechanical defects, contamination, and interface degradation. Developing transfer-free methodologies that enable direct on-chip synthesis therefore marks a critical advancement toward practical implementation of atomically thin circuitry. Controlling the substitution reaction time offers precise tuning of the graphene-to-hBN ratio tailoring the material's electronic properties [2].
This study systematically investigates the temporal dynamics of lateral heterostructure formation via chemical conversion of epitaxial graphene on 6H-SiC (0001) substrates. Pre-grown epitaxial graphene on SiC is exposed under controlled conditions to ammonia and boric acid vapours in an Ar-assisted Chemical Vapour Deposition (CVD) process at 1000 ℃ for varying durations [3]. X-ray photoelectron spectroscopy (XPS), scanning tunneling microscopy (STM), and atomic force microscopy (AFM) measurements are used to confirm the substitution of h-BN domains within the epitaxial graphene layer as a function of reaction time, revealing compositional evolution. Raman spectroscopy is used to confirm defect nucleated nature of the conversion reaction. The temporal control of heterostructure formation demonstrated in this work, combined with the transfer-free synthesis directly on device-compatible SiC substrates, facilitates a scalable route toward rational design of two-dimensional semiconductor materials and implementation of atomically thin circuitry for integrated applications in nanoelectronics.

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Field of Condensed Matter:

Energy and Functional Materials

Materials and devices / 79

Domain Engineering in Epitaxial $BaTiO_3$ Thin Films Toward Integrated Photonics

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Integrating ferroelectric $BaTiO_3$ (BTO) into photonic platforms requires thin films that not only exhibit strong electro-optic behavior but also favour in-plane (a-domain) polarization. However, reliably producing such domain-engineered films remains a challenge due to the complex interplay between strain, stoichiometry, and growth conditions. In this work, we demonstrate a controlled approach to synthesizing epitaxial a-domain–rich BTO thin films on MgO using pulsed laser deposition. By systematically adjusting substrate temperature and oxygen pressure, we uncover a clear and reproducible transition from strained c-domain structures to predominantly a-oriented films, with optimal domain alignment emerging in the 720–760 ℃ and ˜150 mTorr growth window. Structural and spectroscopic measurements show that films grown under these conditions display improved tetragonal ordering, reduced lattice disorder, and smoother surfaces; characteristics that are essential for low-loss optical integration. These domain-optimized BTO films exhibit the structural quality

and ferroelectric orientation needed to unlock strong electro-optic responses in waveguide geometries, providing a practical pathway toward high-performance modulators and photonic components for future integrated and quantum technologies.

Field of Condensed Matter:

Energy and Functional Materials

Superconductivity / **80**

Evolution from charge-order to superconductivity in cuprates

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High-temperature superconductivity in cuprates is achieved through doping Mott insulators, but the critical process underlying the emergence of superconductivity remains unclear. Combining high-resolution resonant inelastic X-ray scattering (RIXS) and scanning tunneling microscopy (STM), we have investigated Bi2Sr2(Ca,Dy)Cu2O8+δ near the onset of the superconducting dome. Our results indicate that Cooper pairs grow out of a charge-ordered insulating state and condense accompanied by an enhanced interplay between charge excitations and electron-phonon coupling [1]. While charge orders (CO) are considered a significant competitor of high-temperature superconductivity in underdoped cuprates, overdoped cuprates have traditionally been viewed as conventional Fermi liquids without collective electronic order. Using Cu L3 edge and O K edge RIXS, we have revealed the presence of CO in overdoped La2-xSrxCuO4 beyond the superconducting dome [2]. Our results suggest that CO is prevalent in the overdoped metallic regime, requiring a reassessment of the traditional understanding of overdoped cuprates as weakly correlated Fermi liquids.

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Field of Condensed Matter:

Superconductivity

Microstructural characterisation / **81**

Photo-Induced Current Transient Spectroscopy of Si/SiO_2 Interface Defects in High-Resistivity Silicon

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Silicon metal-oxide semiconductor (MOS) device structures are vital for realizing quantum computing devices based on single atoms acting as qubits in silicon. These atoms must be located within

˜20 nm of the Si/SiO2 interface to allow proper operation of control electrodes and read-out structures. [1] Qubits store quantum information in electron–nuclear spin states, which are highly sensitive to fluctuating electric and magnetic fields arising from nearby charge and spin defects. Therefore, probing the Si/SiO2 interface quality is crucial, as environmental interactions can induce decoherence. High-resistivity silicon substrates are essential for quantum applications because they minimize parasitic conduction and electromagnetic losses [2]. To study defect states in such substrates, we perform photo-induced current transient spectroscopy (PICTS) on simple source–drain devices implanted with low fluences of Er, H, and P ions. Measurements were carried out using a 780 nm laser diode over a temperature range from 300 K down to 86 K. PICTS probes photo-conductivity decay as a function of temperature, revealing generation–recombination processes in highly resistive semiconductors. This non-invasive technique has high sensitivity to oxide and bulk defects and only requires two ohmic contacts diffused through a layer. As an optically driven technique, PICTS can probe defects at cryogenic temperatures below 4K with photon pulses being used to excited charge carriers across the bandgap to circumvent the carrier freeze-out that occurs at these low temperatures. [3]

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Field of Condensed Matter:

Quantum Materials

Materials and devices / **82**

Probing Interface Defects in MOSFETs for Quantum Applications

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Silicon metal-oxide semiconductor device structures are vital for realizing quantum computing devices based on single atoms acting as qubits in silicon. The atoms forming the qubits must be located within about 20 nm of the Si/SiO2 interface in these devices to allow control electrodes and read-out structures to work. [1] These qubits typically are based on storing quantum information in electron-nuclear spin states and are very sensitive to fluctuating electric and magnetic fields associated with charge and spin defects in the vicinity of the qubit. Probing the quality of the Si/SiO2 interface is crucial for advancing quantum applications, as quantum states are susceptible to decoherence from environmental interactions. This work focuses on the in-house fabrication of metal-oxide-semiconductor field-effect transistors (MOSFETs) and optimizing techniques for probing interface defects at temperatures down to cryogenic temperatures, where quantum devices typically operate. These defects, acting as trapping and scattering centers, influence the functionality and characteristics of the MOSFET devices and this allows these defect states to be probed and quantified. We employ charge pumping (CP) to probe these defects, utilizing substrate current measurements under periodic gate pulses to drive the device between accumulation and inversion states. [2] This method enables precise quantification of trap densities, as well as their energy and spatial distributions, with high sensitivity and simplicity. CP is particularly effective for small-channel MOSFETs, requiring minimal analytical effort and no extensive prior knowledge of defect properties. We report charge pumping measurements on p-channel MOSFETs, both un-implanted and ErO-implanted, to inves-

tigate and compare their interface trap dynamics from room temperature down to liquid nitrogen temperatures.

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Field of Condensed Matter:

Quantum Materials

Topological materials / **83**

Microwave-to-Optical Quantum Transduction Mediated by Magnons: Utilizing Topological Insulators and Antiferromagnets

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The quantum transduction, or equivalently quantum frequency conversion, between microwave and optical photons is a quantum technology that enables the interconnects between quantum devices such as quantum memories and quantum processors. It is also essential for realizing large-scale quantum computers with superconducting qubits. Due to the large frequency difference between microwave and optical ranges, the quantum transduction needs to be done via the interactions between photons and intermediate bosonic modes or via the nonlinear interaction between photons.

In this talk, we focus on the microwave-to-optical quantum transduction mediated by magnons. Earlier studies have so far utilized ferromagnetic magnons in ferromagnets such as YIG. The quantum transduction mediated by magnons can have a wide bandwidth and can be operated even at room temperature, which can be the merits toward practical use of magnon-mediated transducers.

In the first part, we propose a way to improve the transduction efficiency by utilizing the topological Faraday effect of 3D topological insulator thin films that is independent of the sample thickness in the terahertz regime. This leads to a large Faraday rotation angle and therefore enhanced light-magnon interaction in the thin-film limit. We show theoretically that the transduction efficiency between microwave and terahertz photons can be greatly improved from the one with YIG alone by utilizing the heterostructures consisting of topological insulator thin films, such as Bi2Se3 and ferromagnetic insulator thin films, such as YIG.

In the second part, we formulate a theory for the microwave-to-optical quantum transduction mediated by antiferromagnetic magnons in antiferromagnets. We derive analytical expressions for the transduction efficiency in the cases with and without an optical cavity (where a microwave cavity is used in both cases). In contrast to the case of ferromagnets, we find that the quantum transduction can occur even in the absence of an external static magnetic field.

Field of Condensed Matter:

Magnetism

Spectroscopies 1 / **84**

Ultrafast light-matter interaction: from transition metal oxides to van der Waals materials

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In quantum materials, exotic quantum states can emerge as a result of strong many-body interaction that are of charge, magnetic, orbital and structural origins. The delicate balance among these interacting degrees of freedom engenders not only a ground state, but also many other competing metastable states with distinct macroscopic properties. Despite static tuning methods, the rapidly developing ultrafast science has now made it possible to dynamically control quantum materials at an unprecedented level, that is, the direct manipulation of elementary excitations at their fundamental time and energy scales. Here, we show examples on how ultrafast laser excitation can lead to 'hidden'phases in strongly correlated transition metal oxides and Weyl semimetal materials. We also demonstrate, in atomic-thin transition metal dichalcogenides, the strong THz pulse can prompt quantum tunneling transport of excitons on the femtosecond timescale.

Field of Condensed Matter:

Quantum Materials

85

Tuneable Negative Thermal Expansion in Fe/Cr-Substituted Nd2Co17 Compounds via Magnetoelastic Coupling

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The development of materials with precisely tuneable thermal expansion is critical for high-precision applications, yet achieving composition-dependent bidirectional switching between positive and negative thermal expansion (NTE) remains a key challenge. Here, we present a magnetoelastic approach to tailor anisotropic thermal expansion in Nd2(Co1-xFex)17-yCry compounds. Synchrotron X-ray diffraction studies reveal that increasing Fe content induces a reversible lattice response, while Co-rich compositions (e.g., Nd2(Co0.5Fe0.5)13.7Cr3.3) display conventional positive expansion, Fe-rich variants (e.g., Nd2(Co0.2Fe0.8)14.7Cr2.3) exhibit pronounced uniaxial NTE along the c-axis (αc = -5.23×10-6 K-1) below the Curie temperature (TC). This transition originates from strong magnetoelastic coupling at specific crystallographic sites, where Fe occupancy at the 6c Wyckoff position enhances negative exchange interactions, driving c-axis contraction via magnetostriction.

Compositional tunning not only suppresses the volume expansion coefficient (reducing αV by 20% at x = 0.7) but also modulates TC (442 - 625 K). Critical exponent (β, γ, δ) analyses near TC aligns with mean-field theory, confirming the dominant role of long-range magnetic interactions. Our findings establish a new strategy for achieving zero or near-zero thermal expansion in rare-earth intermetallic, making these materials promising candidates for precision thermal management.

We acknowledge and appreciate support from the Australian Research Council, the Australian Synchrotron and ANSTO.

Field of Condensed Matter:

Magnetism

Topological materials / **86**

Unveiling Anisotropic Electronic Transport in Kagome Metal $YbCo_6Ge_6$

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Kagome materials, notable for their unique band structure characterized by flat bands, Dirac cones, and van Hove singularities (or saddle points), coupled with a geometrically frustrated lattice, provide an exceptional platform for exploring emergent quantum phenomena, including topological phases, strongly correlated electron systems, and magnetic ordering. Among these, the Kagome metal $YbCo_6Ge_6$ crystallizes in a hexagonal structure (space group, P6/mmm) and exhibits a fascinating interplay of properties. While paramagnetic, its negative Curie-Weiss temperature and effective magnetic moment close to Yb^{3+} hint at potential antiferromagnetic interactions [1]. Magnetotransport along the a-axis reveals strong negative magnetoresistance (NMR), attributed to the Kondo effect [2]. At the same time, a speculated charge density wave (CDW) at 95 K induces a doubling of unit cells along the c-axis and in-plane distortions of the Co-Kagome lattice [3]. Recent theoretical studies highlight two high-order saddle points (HOSP) near the Fermi level, creating flat bands that amplify correlation effects and foster electronic instabilities [4]. These unique properties of $YbCo_6Ge_6$ make it an intriguing system for further exploration.

In this talk, we report on $YbCo_6Ge_6$ single crystals grown using a Sn flux. We found a striking anisotropy in the longitudinal resistivity between the current applied in the Kagome plane (ab-plane) and along the c-axis. This result is likely linked to the flat bands generated by HOSP near the Fermi level. Additionally, we observed Kondo effect-assisted negative magnetoresistance (NMR) in the interplane transport. Second-harmonic transport measurements unveiled an anisotropic nonlinear Hall effect (NLHE); the origin of this effect will be discussed. These observations position $YbCo_6Ge_6$ as a compelling platform for studying flat band-driven transport phenomena alongside artificially engineered systems like magic-angle twisted bilayer graphene [5]. Our work underscores the material's potential for advancing the understanding of correlated electron systems and topological states, paving the way for future explorations in quantum materials.

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Field of Condensed Matter:

Topological Materials

Materials under extreme conditions / **87**

Melting of Noble Gases under Extreme Conditions and Machine Learning Structural Analysis

Author: Tiantian Yu[None]

The melting transitions of light noble gas crystals in extreme conditions are investigated using Monte Carlo simulations. Helium, neon and argon are put under a series of pressures up to 100 GPa, a million times the atmosphere pressure, combined with no magnetic field, or a strong magnetic field of 0.30 a.u.. We use a parallel-tempering implementation of the MC method (PTMC) written in the modern computer language Julia: Several MC runs are distributed over the whole temperature range of interest and are performed in parallel to enable ergodic simulations. Simulation boxes of different shapes are implemented to treat different crystal structures (fcc, hcp and bcc) on equal footing.
The melting points are obtained under such extreme conditions. The pressure-melting point relationship with no magnetic field is compared with various previous studies.
When the magnetic field is switched on, the melting points of light noble gas crystals increase significantly under low pressure. As the pressure increases, the difference in melting points between the field-free and strong magnetic field cases shrinks and becomes less distinct.
To study the structures and phase transitions of noble gas crystals, especially the possible fcc-to-hcp or hcp-to-fcc transitions, structural analysis methods based on common neighbour analysis (CNA) and machine learning are developed.

Field of Condensed Matter:

Magnetism

Magnetism / **88**

Confinement-driven renormalization of magnon and phonon spectra in Fe3O4 nanoparticles

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Magnetite (Fe_3O_4) nanoparticles exhibit pronounced size-dependent magnetic and thermal properties relevant to spintronics, thermoelectrics, biomedical heating, and catalytic applications. In bulk Fe_3O_4, magnons and phonons govern key behaviours such as the Verwey transition, spin-lattice coupling, and thermal transport. However, at the nanoscale, their behaviour remains poorly understood due to the combined influence of finite-size confinement, surface strain, and heterogeneous exchange interactions. Despite extensive interest in nanoscale magnetism, a unified framework linking particle size to quasiparticle renormalisation has yet to be established.

In this presentation, I will show how time-of-flight inelastic neutron scattering, combined with molecular dynamics and linear spin-wave theory, resolves the full magnon and phonon renormalisation across Fe_3O_4 nanoparticles ranging from 100 nm (bulk-like) to 8 nm. We find that nanoscale confinement universally alters quasiparticle dynamics: optical phonons soften by ~ 0.5 meV and broaden significantly due to surface-induced strain, while acoustic magnons display a pronounced 36\% reduction in group velocity (14\,000 $\rightarrow$ 10\,000 m s^{-1}) arising from bond-angle disorder. These magnetic excitations are quantitatively described by a heterogeneous exchange model comprising bulk-like interactions (J) and weakened surface interactions ($J' = 0.7J$), which collectively account for the observed spectral broadening and magnon softening.

These results establish finite-size confinement as a general mechanism for renormalising vibrational and spin excitations in strongly correlated oxides. By directly connecting surface strain and exchange disorder to measurable changes in quasiparticle spectra, this work provides a foundation for engineering spin-wave coherence in spintronic devices and tailoring phonon transport in thermoelectric materials. The principles demonstrated here extend broadly to functional oxides such as

$CoFe_2O_4$ and Mn_3O_4, offering a pathway for the rational design of nanoscale materials with tuneable magnetic and thermal properties.

Field of Condensed Matter:

Magnetism

Nanoparticles / **89**

Tuning the Surface States of Fe3O4 Nanoparticles for Enhanced Magnetic Anisotropy and Induction Heating Efficacy

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Magnetite (Fe_3O_4) nanoparticles are central to biomedical technologies such as magnetic hyperthermia, targeted drug delivery, and MRI contrast enhancement, owing to their biocompatibility, superparamagnetism, and ability to generate heat under alternating magnetic fields. A key challenge, however, lies in understanding how surface chemistry, particularly adsorbed water and hydroxyl groups, influences magnetic relaxation processes and induction heating performance. Although surface water is ubiquitous in nanoparticles, its precise impact on magnetic anisotropy, spin dynamics, and the specific absorption rate (SAR) remains poorly resolved.

In this presentation, I will show how tuning the surface states profoundly modifies the magnetic response of 8 nm Fe_3O_4 nanoparticles. Through synchrotron diffraction, thermogravimetric analysis, X-ray photoelectron and absorption spectroscopy, and time-of-flight inelastic neutron scattering, we reveal that heat treatment removes surface water and FeOOH species, forming a γ-Fe_2O_3 shell. AC magnetic susceptibility measurements demonstrate that this surface modification suppresses the low-temperature clustered spin-glass transition, increases the blocking temperature, and enhances the magnetic anisotropy while reducing the spin relaxation time. These changes lead to a 140\% increase in the SAR, directly linking surface chemistry to induction heating efficiency.

These results establish surface-state engineering as a powerful route to optimising Fe_3O_4 nanoparticles for biomedical heating applications and provide a mechanistic framework for controlling magnetic anisotropy and relaxation dynamics through targeted surface modification.

Field of Condensed Matter:

Magnetism

Magnetism / **90**

Materials chemistry of partial spin-liquids and other “idle spin” states

Author: Chris Ling[1]

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At very low temperatures, theoretically down to 0 K, the unpaired electronic spins on magnetic ions arranged in "frustrated"topologies such as triangles have difficulty finding long-range ordered ground states. This ideally leads to a Kitaev quantum spin-liquid (QSL) state in which the spins continue to fluctuate so the compound has finite entropy at absolute zero. QSL compounds have been intensively studied by the condensed-matter physics community, mostly from theoretical/computational perspectives because there are so few experimental realisations. This presentation will focus on *partial* spin liquids, in which some of the spins resolve into long-range order but others do not. These have attracted much less theoretical interest than full QSLs, but may be more common in the real world. It will highlight examples from our own work and reported cases that have languished in the literature for want of a unified way to describe them. It will include some crystal-chemical design principles, physical properties, and means to study their complex magnetic structures such as polarised neutron total-scattering and inelastic neutron spectroscopy combined with *ab initio* computational modelling.

Field of Condensed Matter:

Magnetism

Condensed matter theory / **91**

Strange diffusivity and incoherent transport on approach to an antiferromagnetic insulator

Authors: Youngmin Eom[1]; Igor S. Tupitsyn[2]; Nikolay V. Prokof'ev[2]; Boris Svistunov[2]; Evgeny Kozik[3]; Aaram Kim[1]

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We study charge transport across the metal-to-insulator crossover of the half-filled two-dimensional Hubbard model with controlled accuracy. The dynamical current-current correlation function is evaluated directly in the thermodynamic limit, and the optical conductivity is obtained by numerical analytic continuation. Our multiscale scheme combines unbiased diagrammatic Monte Carlo at low frequencies with a self-consistent semi-analytic diagrammatic treatment at high frequencies. Over a broad temperature range where the DC resistivity follows anomalous scaling, the simple Nernst-Einstein relation yields the diffusivity with the characteristic~1/\sqrt{T} "strange metal"behavior. It was also revealed that the insulating regime is entered through a peculiar non-Fermi liquid state —which we call a Pseudogap Metal—characterized by insulating charge compressibility coexisting with metallic transport while the one-particle self energy captures a significant anisotropy. Diagrammatically, we shows that the high-temperature incoherent transport is captured by the dressed polarization bubble, whereas near the metal-insulator crossover, the effective interaction vertex between opposite-spin particles is responsible for transferring the Drude weight to a high-frequency continuum.

Field of Condensed Matter:

Quantum Materials

Magnetism / **92**

Unconventional magnetism probed by polarised neutron spectroscopy

Author: Yusuke Nambu[None]

Unconventional magnetism often emerges when the chiral degree of freedom of spins becomes decisive beyond simple collinear order. In this talk, I will show how polarised neutrons directly access the chiral term, enabling sign-resolved determination of spin chirality in both static magnetic structures and reversibly switched states under external perturbations. Next, I will visualise the opposite polarisations —the handedness of spin precession —of low- and high-energy magnon branches, even in collinear magnets, and account for the characteristic temperature dependence of spin-current signals. I will then turn to frustrated triangular-lattice antiferromagnets, where vector-chiral correlations provide a topological route to long-lived fluctuating states without long-range order. Together, these results unify chirality and momentum-dependent magnon polarisation into a microscopic framework for engineering unconventional magnetic responses and robust spin transport.

Field of Condensed Matter:

Magnetism

Superconductivity / **93**

Discovery of Segmented Fermi Surface in a Superconductor

Author: Hao Zheng[1]

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Since the early days of Bardeen-Cooper-Schrieffer theory, it has been predicted that a sufficiently large supercurrent can close the energy gap in a superconductor and create gapless Bogoliubov quasiparticles through the Doppler shift of quasiparticle energy due to the Cooper pair momentum[1]. In this gapless superconducting state, zero-energy quasiparticles reside on a segment of the normal state Fermi surface, while its remaining part is still gapped. However, the segmented Fermi surface of a finite-momentum state carrying a supercurrent has never been detected directly. We use quasiparticle interference (QPI) technique to image field-controlled Fermi surface of Bi2Te3 thin films proximitized by the superconductor NbSe2. By applying a small in-plane magnetic field, a screening supercurrent is induced which leads to finite-momentum pairing on topological surface states of Bi2Te3[2]. Our measurements and analysis reveal the strong impact of finite Cooper pair momentum on the quasiparticle spectrum, and thus pave the way for STM study of pair density wave and FFLO states in unconventional superconductors.

[1] Phys. Rev. 137, A783-A787 (1965)
[2] Science 374, 1381-1385(2021)

Field of Condensed Matter:

Superconductivity

Magnetism / **94**

Probing Vibronic Spin-Lattice Dynamics in the Frustrated Pyrochlore $Tb_2Ti_2O_7$ Using Free Electron Laser based THz Pump–Probe Spectroscopy

Author: Evan Constable[1]

Co-authors: C. Decorse ; R. Ballou ; S. De Brion ; Y. Alexanian ; Z. Wang

[1] *ANSTO - Australian Synchrotron*

The rare-earth pyrochlore $Tb_2Ti_2O_7$ (TTO) remains one of the most puzzling frustrated magnetic systems. Although its crystal-electric-field (CEF) scheme and exchange topology nominally favour a classical dipolar spin-ice state, neither spin-ice order nor any long-range magnetism emerges down to tens of millikelvin. Increasing evidence points to the decisive role of magneto-elastic interactions, where hybridisation between the non-Kramers Tb^{3+} CEF levels and low-energy phonons generates a vibronic coupling that can melt dipolar order and promote quadrupolar degrees of freedom. This competition has been proposed to stabilise either a quadrupolar-ice-like state or a vibronic quantum spin liquid, sensitively dependent on stoichiometry. Understanding how such spin-lattice entanglement shapes the low-temperature phase remains an outstanding challenge.
Magneto-optical THz spectroscopy has played a central role in developing this picture by resolving the fine structure and symmetry breaking in the first excited CEF manifold. Under applied magnetic field, these levels split in characteristic ways that reveal the underlying anisotropies induced by the lattice. Building on this foundation, we employ polarisation-resolved pump–probe spectroscopy at the ELBE free-electron laser to selectively drive the vibronically coupled Tb^{3+} excitations with intense 0.7 THz pulses, while tracking the induced magnetisation through ultrafast optical Faraday rotation. This approach enables us to follow, in real time, the decay of individually excited Tb ions within the primitive cell and potentially disentangle linear and nonlinear magnetic responses linked to the hybrid CEF–phonon modes.
To interpret the observed relaxation channels, and field-dependent oscillations, we model the Tb^{3+} single-ion dynamics using modern quantum-optical frameworks implemented in QuTiP. Direct comparison between experiment and theory provides new insight into the microscopic vibronic processes that may underpin quadrupolar frustration and the emergence of unconventional spin-liquid physics in $Tb_2Ti_2O_7$.

Field of Condensed Matter:

Magnetism

Microstructural characterisation / **95**

Fabrication and characterisation of low-dimensional materials on surfaces

Author: Jennifer MacLeod[1]

[1] *Queensland University of Technology*

The bottom-up construction of materials on solid surfaces has emerged as a powerful strategy for tailoring nanostructures with unique properties. Our research explores the synthesis and characterization of one dimensional (1D) and two dimensional (2D) materials on atomically well-defined surfaces, which serve as supports, templates, and catalysts for chemical reactions. We employ molecular self-assembly, on-surface reactions of atomic and molecular building blocks, semiconductor heteroepitaxy and the growth or transfer of 2D materials under ultrahigh vacuum conditions to fabricate novel materials systems. Using atom scale measurements with scanning probe microscopy, complemented by density functional theory modelling and photoemission spectroscopy, we aim to uncover the mechanisms that govern structure and properties at the nanoscale. In this talk, I will present our recent advances in fabricating and characterizing low dimensional materials, highlight opportunities enabled by ultrahigh vacuum transfer of 2D materials onto clean, ordered surfaces, and discuss how these systems open new avenues for observing quantum phenomena.

Field of Condensed Matter:

Quantum Materials

96

Local magnetism in the face-sharing Mn_3O_{12} trimer family $Ba_4MMn_3O_{12}$

Author: Maria Sanchez Echeverria[1]

[1] *University of Sydney*

High-performance magnets are dominated by rare-earth (RE) compounds, despite environmental and economic costs. Developing sustainable alternatives is urgent, and our work targets transition metal (TM)–based systems.
The $Ba_4MMn_3O_{12}$ family (M = TM or RE) crystallizes in R-3m symmetry with face-sharing M_3O_{12} trimers that host competing ferro- and antiferromagnetic interactions, leading to unusual properties. Prior studies reported low-temperature magnetic transitions, but the microscopic magnetic ordering remains unclear.
We synthesized $Ba_4MMn_3O_{12}$ (M = Nb, Ta, Sb) and reproduced bulk magnetization and heat capacity results, confirming low-temperature magnetic ordering. Effective magnetic moments are smaller than expected for free spins, implying strong inter-trimer coupling or cluster formation. Two scenarios have been proposed: partial cancellation of localized spins, or an itinerant electron delocalized across the trimer. Dynamic susceptibility measurements are underway to distinguish between them. Interestingly, we also find the magnetism strongly depends on thermal history, a feature not previously noted.
To resolve the local structure, we employed neutron powder diffraction. For M = Nb and Ta, the data reveal long-range antiferromagnetic order with propagation vector k = (3/2, 0, 0) and magnetic space group $PA2_1/c$. Strikingly, one Mn per trimer appears non-magnetic, consistent with exotic "idle spin"states seen in other frustrated systems.
We will present combined Rietveld refinement, powder neutron diffraction and diffuse scattering analysis to establish a comprehensive picture of magnetism in this family.

Field of Condensed Matter:

Magnetism

Condensed matter theory / 100

Exact Spectral Properties of Fermi Polarons in One-Dimensional Lattices

Author: XiaJi LIU[1]

Co-authors: Hui Hu ; Jia Wang

[1] *Swinburne University of Technology*

We calculate the exact spectral function of a single impurity repulsively interacting with a bath of fermions in one-dimensional lattices, by deriving the explicit expression of the form factor for both regular Bethe states and the irregular spin-flip state and ⍰-pairing state, based on the exactly solvable one-dimensional Hubbard model. While at low impurity momentum ⍰ ~0 the spectral function is dominated by two power-law Fermi singularities, at large momentum we observe that the two singularities develop into two-sided distributions and eventually become anomalous Fermi singularities

at the boundary of the Brillouin zone (i.e., ☒=±☒), with the power-law tails extending toward low energy. Near the quarter filling of the Fermi bath, we also find two broad polaron peaks at large impurity momentum, collectively contributed by many excited many-body states with non-negligible form factors. Our exact results of those distinct features in one-dimensional Fermi polarons, which have no correspondences in two and three dimensions, could be readily probed in cold-atom laboratories by trapping highly imbalanced two-component fermionic atoms into one-dimensional optical lattices.

Field of Condensed Matter:

Theory

Magnetism / **101**

Continuous collapse of the spin cycloid in multiferroic BiFeO3 thin films under an applied magnetic field probed by neutron scattering

Author: Clemens Ulrich[1]

Co-authors: Md. Firoz Pervez [1]; Zhang Zhang [2]; Yen-Lin Huang [2]; Lucas Caretta [3]; Ramamoorthy Ramesh [4]

[1] *University of New South Wales*

[2] *Lawrence Berkeley National Laboratory*

[3] *Brown University*

[4] *University of California, Berkeley*

Bismuth ferrite (BiFeO3) is one of the rare materials which exhibits multiferroic properties already at room temperature. Therefore, it offers tremendous potential for future technological applications, such as in low-energy, high-density data storage or logic devices in IT. BiFeO3 possesses a G-type antiferromagnetic structure, where the Fe3+ spins form an incommensurate spin cycloid. Exploring and understanding the effects of an electric field, magnetic field, strain and film thickness allows for the manipulation of the spin cycloid and is therefore of major interest for future technologies. By performing neutron diffraction experiments using the triple-axis instrument Taipan at ANSTO we have determined that the spin cycloid can be systematically suppressed at an applied magnetic field of 10 T in a BiFeO3 thin film of 100 nm thickness grown on a (110)-oriented SrTiO3 substrate [1]. As predicted by theoretical calculations, we observed that the required critical magnetic field to suppress the spin cycloid in a BiFeO3 thin film was significantly lower as compared to the previously reported critical magnetic field for bulk BiFeO3. Furthermore, in contrast to bulk single crystals, the spin cycloid in the BiFeO3 thin film continuously expands with increasing magnetic field before the complete transformation into a G-type antiferromagnetic spin order. Such tuning of the length of the spin cycloid up to its complete suppression offers further functionalities for future applications in spintronics or magnonics.
[1] Md. Firoz Pervez, et al., Phys. Rev. B 111, 174426 (2025).

Field of Condensed Matter:

Magnetism

102

Application of Artificial Intelligence to Calculate Electrostatic Interaction in Molecular Dynamics Simulation of Charged Parti-

cles

Author: Pyeong Jun Park[1]

[1] *Korea National University of Transportation*

Molecular Dynamics (MD) simulations are indispensable tools for exploring the structural, dynamic, and thermodynamic properties of complex systems, particularly those involving charged particles like proteins, nucleic acids, and ionic liquids. However, the calculation of long-range electrostatic interactions, typically handled by methods such as Particle Mesh Ewald method, remains the most computationally demanding component. This bottleneck severely limits the system size and timescale accessible to conventional MD. This study proposes a development and application of Artificial Intelligence (AI) models, specifically Neural Networks and deep learning architectures, to create efficient surrogate models for predicting electrostatic energies. The AI model is trained on pre-calculated high-fidelity electrostatic data from various molecular configurations. The goal is to capture the non-local dependencies inherent in the charge distribution and interaction environment with minimal computational overhead. Successful implementation promises to unlock the simulation of systems at long timescales, fundamentally advancing the scope of computational material science and biomolecular discovery.

Field of Condensed Matter:

Biophysics and medical applications

Superconductivity / **103**

Electronic structures and superconductivity of new RP-type nickelate superconductors

Author: DAOXIN YAO[None]

The recently discovered Ruddlesden-Popper bilayer superconductor La3Ni2O7 has attracted widespread attention due to its high Tc˜80 K under a pressure. Soon after that, the trilayer La4Ni3O10 was found to show superconductivity at high pressure too. Our density functional theory calculations indicate that the 3dx2−y2 and 3dz2 orbitals of Ni cations mixing with oxygen 2p orbitals play critical role in the emergence of superconductivity in the bilayer and trilayer nickelate superconductors, especially the apical oxygen ions forming the Ni–O–Ni bonds. We propose a bilayer two-orbital model for La3Ni2O7 under high pressure, primarily based on the 3dx2−y2 and 3dz2 orbitals of Ni. Through Wannier downfolding and symmetry analysis, we obtain parameters such as electron hopping and site-energy, which provide an excellent description of the electronic band structure and Fermi surface. To explicitly consider the physics of O-p orbitals, we further introduce a higher energy model (11-orbital model). Based on these models, we study the charge transfer, Zhang-Rice singlet bands, pairing symmetry, and superconducting transition temperature in La3Ni2O7. We obtain a comprehensive superconducting phase diagram in the doping plane and find that the La3Ni2O7 under pressure is situated roughly in the optimal doping regime of the phase diagram. We perform a first-principles study of La4Ni3O10 for both the P21/a phase at ambient pressure and I4/mmm phase at high pressure. Our results show the characteristic upward shift of a Ni-3dz2 bonding band under pressure in La4Ni3O10. We propose a trilayer two-orbital model by performing Wannier downfolding on Ni-eg orbitals. According to the model, our calculated spin susceptibility under RPA shows that the 3dx2−y2 orbital is also important for the magnetic fluctuation in the RP series. Moreover, a high energy 16-orbital model with direct dp, pp hoppings is proposed, which implies that La4Ni3O10 also lies in the charge-transfer picture. Our exposition of electronic reconstructions, multiorbital models and superconductivity shed light on theoretical electronic correlation study and experimental exploration of superconductors in the RP series.

Field of Condensed Matter:

Superconductivity

104

Magnetic properties of mixed manganese selenites Mn3A2(SeO3)6 (A = Sc, Fe)

Authors: Artem Moskin[1]; Chris Ling[1]

[1] *The University of Sydney*

Pushing the boundaries of exotic properties (i.e. spintronics and superconductivity) requires discovering new materials. A promising route is to investigate classes of materials that were previously overlooked due to structural complexity. One of such group is mixed 3d-metals selenites. The selenite group SeO32- possesses a stereochemically active lone pair of electrons which leads to reduced dimensionality by restricting some exchange interactions between magnetic atoms. The structure [1] of Mn3Fe2(SeO3)6 has the space group Pna21 which is noncentrosymmetric and polar, leading to potential multiferroic properties.
In Mn3Fe2(SeO3)6 the Mn ions form a distorted square plane through vertices and corner sharing oxygen links with Mn-O-Mn angles of 103-123° which should lead to a mixture of ferro- and antiferromagnetic exchange interaction. These square planes are decorated with Fe octahedra, and layers are interconnected through the selenite groups. Mn3Sc2(SeO3)6 is isostructural with slightly bigger unit cell parameters. Both compounds were synthesized by a hydrothermal method.
According to our magnetic measurements, Mn3Fe2(SeO3)6 orders magnetically below TN1 = 34 K and TN2 = 10 K, while the magnetic susceptibility above the transition can be fit to a Curie-Weiss law with θ = -116 K and μ_eff = 13.54μ_B. These parameters lead to a frustration index of 116/34 = 3.4. The scandium analogue Mn3Sc2(SeO3)6 shows transition signatures at 2.5 K, while the paramagnetic state gives θ = -34 K and μ_eff=10.21μ_B, with frustration index increased to 18. Thus, we propose that most of the antiferromagnetic interactions are incurred by Mn-Fe pairs rather than Mn-Mn. Additionally, on the M(H) curve, two anomalies were observed around 1.1 T and 5.5 T. With DFT calculation analysis it was proposed that Mn3Fe2(SeO3)6 consist of antiferromagnetically ordered ferromagnetic stripes, while Mn3Sc2(SeO3)6 contain ferromagnetic trimers with checkerboard type ordering.
[1] G. Giester, Bull. of Chem. Soc. of Japan, (93) 5, 2020

Field of Condensed Matter:

Magnetism

Condensed matter theory / 105

Viscous stress causes giant magnetoresistivity in liquid metals

Author: Jack Engdahl[1]

[1] *UNSW*

We theoretically study the response of liquid metal to external electric and magnetic fields to explain the experimentally observed giant magnetoresistivity measured in liquid metals which is not
observed in the solid state. For simplicity we consider a coaxial conducting cylinder geometry with insulating base and roof. We argue that the correct application of electron transport theory must be performed in the proper reference frame of the fluid. By constructing a model based on viscous magnetohydrodynamics and Ohmic transport, we show that magnetic field dependent viscous dissipation greatly contributes to the resistivity of the liquid metal. Our theoretical prediction of magnetoresistivity for liquid Gallium agrees well with experimental observation.

Field of Condensed Matter:

Theory

Materials and devices / 106

low-cost high efficiency oxide-based thermoelectric materials and device

Author: Yannan Lu[1]

Co-authors: Daniel Liang [1]; Nazrul Islam [1]

[1] *CSIRO*

Thermoelectric (TE) oxide materials have attracted significant interest due to their abundance, low-cost processing, and excellent thermal and chemical stability. However, their relatively low conversion efficiency has remained a major barrier to practical applications. In this work, several cost-effective oxide-based thermoelectric materials are investigated, along with the segmentation of oxide and semimetal materials. By combining the advantages of both material types, segmented legs with high efficiency and high-temperature stability can be developed. Materials for segmentation are selected based on their compatibility factors and an "efficiency ratio"that balances conversion efficiency with material cost. Numerical modelling results show that conversion efficiencies exceeding 10% can be achieved for unicouples using segmented legs comprising p-type $Ca_3Co_4O_9$ and n-type ZnO oxides, excluding electrical and thermal losses. These results provide valuable guidance for designing low-cost, high-efficiency thermoelectric modules based on oxide materials.

Field of Condensed Matter:

Energy and Functional Materials

Magnetism / 109

Detection of magneto electric multipoles with spherical neutron polarimetry

Author: Jian-Rui Soh[1]

Co-authors: Andrea Urru [2]; Anne Stunault [3]; Bertrand Roessli [4]; Henrik Ronnow [5]; Navid Qureshi [3]; Nicola Spaldin [2]

[1] *A*STAR*

[2] *ETHZ*

[3] *ILL*

[4] *SINQ*

[5] *EPFL*

The fundamental interaction between the neutron dipolar field and the magnetization density surrounding the scattering ion, lies at the heart of magnetic neutron diffraction. However, if the ion resides in an environment which breaks both time and spatial inversion symmetry, the current formalism for magnetic diffraction does not fully account for all the possible scattering mechanisms arising from the asymmetry of the magnetization density cloud of the scatterer.

In our work, we have extended the theory of magnetic neutron diffraction to include these effects. Drawing analogies from the magneto-electric (ME) phenomena and standard magnetic neutron

diffraction, developed a framework to calculate the associated ME form factor, size of the ME multipoles and the ME propagation vector from density functional theory (DFT) calculations.

Furthermore, we have identified several material systems, which can not only host these ions but also display an ordered arrangement of these magneto-electric multipoles. Alongside our DFT calculation of the corrections to the scattering amplitudes and form factor of these multipoles, we used spherical neutron polarimetry to provide evidence for the interactions between neutrons and the long-ranged order of these magneto-electric multipoles in CuO.

Field of Condensed Matter:

Magnetism

Superconductivity / **110**

Phenomena and properties in pressurized high-Tc superconducting oxides

Author: Liling Sun[1]

Co-author: Tao Xiang [2]

[1] *Center for High Pressure Science & Technology Advanced Research*

[2] *Institute of Physics, Chinese Academy of Sciences*

Phenomena and properties in pressurized high-Tc superconducting oxides
Liling Sun1,2

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The exploration of emerging phenomena and physics in high-temperature (Tc) superconducting materials from metal oxides has been a frontier topic in condensed matter physics. Particularly, the development of various experimental techniques has opened new opportunities to unravel key issues in this field. Given the nature of strong electron correlation and diverse degrees of freedom inherent in high-Tc superconducting materials, the application of pressure frequently unveils new insights. In this talk, I will report novel phenomena observed from our high-pressure investigations on high-Tc superconducting oxides. These include the pressure-induced crossover from two-dimensional to three-dimensional superconducting states [1] and quantum phase transitions [2] in bismuth-based cuprate superconductors; the pressure-induced superconducting-insulating phase transition in Ba1-xKxBiO3 bismuthates [3]; and signatures of a Lifshitz transition in pressurized electron-doped cuprate [4].

- These woks were in collaboration with GD Gu, CT Lin, SL Li, Q Wu, XJ Zhou, T Xiang.

References：
[1] J Guo and L Sun et al, Nature Physics 16. 295 (2020).
[2] YZ Zhou and L Sun et al, Nature Physics 18, 406 (2022).
[3] JY Han and L Sun et al, Phys. Rev. B 111, L020509 (2025).
[4] JY Zhao and L Sun et al, arXiv 2025

Field of Condensed Matter:

Superconductivity

Magnetism / **111**

Detecting the half-metallic electronic states in Heusler alloys

Author: Rie Umetsu[1]

[1] *Tohoku University*

Since half-metallic electronic structures were theoretically predicted in some half-Heusler and full-Heusler alloys, the half-metallic ferromagnets have been intensively investigated in a field of spintronics. Soft X-ray resonant inelastic X-ray scattering (RIXS) and the magnetic circular dichroism (MCD) were performed in order to detect the half-metallic electronic states in Heusler alloys. Because the RIXS is a photon-in/photon-out spectroscopy technique using a high-brilliance synchrotron light source, it allows us to probe the electronic structures in an elemental specific way by tuning the incoming photon energy to the core-level absorption edges. The MCD in the RIXS spectra can probe the spin-polarized electronic structures due to the strong selection rule of the dipole-allowed transition.
The RIXS-MCD measurements were performed at SPring-8 BL07LSU HORNET using left and right circularly polarized light. Single crystals of some Heusler alloys were grown by the Bridgeman method. The crystal orientation was checked using Laue's back reflection method and the specimen was cut into stripes in the direction parallel to the <100>.
In Mn2VAl and Co2MnSi, it was found that the Zeeman energy, width of the gap formed at the Fermi level, and which spin band opens the half-metallic gap can be revealed from comparison between experimental and theoretical spectra of RIXS-MCD. Furthermore, the RIXS-MCD experiments at the new synchrotron facility in Japan, NanoTerasu, were performed for Co2MnGa alloy, which has been known as a Weyl ferromagnet. Because of the brilliant light at NanoTerasu and the higher resolution of spectra, clearer structures could be observed especially in Co-L edge comparing with the previously obtained spectra at SPring-8. Interestingly, it was found that the Mn-3d orbitals behave half-metallic character around the Fermi level, on the contrary, the Co-3d ones exhibit metallic band character at both spin states. These findings suggest that the Weyl crossing would be caused by the Co-3d electrons.

Field of Condensed Matter:

Magnetism

Superconductivity / **113**

Evidence of P-wave Pairing in K2Cr3As3 Superconductors from Phase-sensitive Measurement

Author: Jie Shen[1]

[1] *Institute of physics, Chinese Academy of Sciences*

P-wave superconductors hold immense promise for both fundamental physics and practical applications due to their unusual pairing symmetry and potential topological superconductivity. However, the exploration of the p-wave superconductors has proved to be a complex endeavor. Not only are they rare in nature but also the identification of p-wave superconductors has been an arduous task in history. For example, phase-sensitive measurement, an experimental technique which can provide conclusive evidence for unconventional pairing, has not been implemented successfully to identify p-wave superconductors. Here, we study a recently discovered family of superconductors, A2Cr3As3 (A = K, Rb, Cs), which were proposed theoretically to be p-wave superconductors. We fabricate superconducting quantum interference devices (SQUIDs) on exfoliated K2Cr3As3, and perform the phase-sensitive measurement. It reveals the admixture of 0- and π-phase in these SQUIDs, and we conclude that the existence of the π-phase is in favor of the p-wave pairing symmetry in K2Cr3As3.
Ref: arXiv:2408.07342

Field of Condensed Matter:

Superconductivity

Superconductivity / **114**

Spin spirals versus spin stripes in underdoped cuprate superconductors: muon spin relaxation data confirms spirals and is inconsistent with stripes

Author: Oleg Sushkov[1]

[1] *University of New South Wales*

All cuprate superconductors are based on doping of parent Mott insulators which are collinear antiferromagnets. With doping by holes or electrons the insulator becomes a poor conductor, called a "pseudogap metal" or a "Mott metal", that supports unconventional high temperature superconductivity.

It is well established in neutron scattering that with doping by holes the systems develop incommensurate spin ordering. The ordering can be static, quasistatic, or dynamic (nematic state). The ordering period is proportional to doping and generally is incommensurate with the lattice. There is no doubt that the ordering is a fundamental property of the pseudogap state that must be understood.

There are two competing models (visualizations) of the ordering, (i) spin stripes and (ii) spin spirals. Experiments with polarized neutrons were inconclusive to distinguish between these models. The cuprate $La_{2-x}Ba_xCuO_4$ ($x = \frac{1}{8}$) plays a special role in the story because the elastic neutron scattering in this case is especially strong indicating large static magnetic moment. The static moment is large because the generally incommensurate structure in this compound is commensurate with period 8 lattice spacing and hence pinning to the lattice suppresses spin quantum fluctuations.

The large static magnetic moment allows us to use μSR to distinguish between the spirals and the stripes. I perform analysis of available μSR data and show that the data is consistent with spin spirals and inconsistent with spin stripes. I also determine value of the magnetic moments in the spin spiral.

Field of Condensed Matter:

Magnetism

Superconductivity / **116**

Interaction of ferroelectric and superconductivity in YBCO/BaTiO3 films

Authors: Golrokh Akhgar[1]; Louis Oppong-Antwi[1]

Co-authors: Peggy Zhang [1]; Nagarajan Valanoor [2]; David Cortie [3]; Wendy Purches [4]

[1] *CSIRO*

[2] *UNSW*

[3] *ANSTO*

[4] *DeteQT*

Epitaxial heterostructures combining superconducting $YBa_2Cu_3O_{7-\delta}$ (YBCO) and ferroelectric $BaTiO_3$ (BTO) provide a platform to probe interfacial coupling relevant to tunable oxide and quantum devices. In this study, YBCO and BTO thin films were grown on $SrTiO_3$ (001) by pulsed laser deposition. X-ray diffraction/reflectometry and atomic force microscopy confirm high-quality, c-axis-oriented epitaxy with smooth, well-defined interfaces. Transport measurements show a reduction of the superconducting transition temperature from ˜86 K in single-layer YBCO to ˜73 K in YBCO/BTO/YBCO trilayers, consistent with interfacial coupling effects (e.g., strain, oxygen stoichiometry, and charge redistribution) associated with the ferroelectric layer. Piezoelectric force microscopy demonstrates robust, reversible ferroelectric switching in both single-layer and heterostructure films. Neutron (polarized) reflectometry resolves the buried interfaces, confirming structural integrity and indicating a weak induced magnetic response within the heterostructure. Together, these results establish YBCO/BTO heterostructures as versatile platforms for reconfigurable, low-power oxide electronics.

Field of Condensed Matter:

Quantum Materials

Quantum science & technology / **117**

The whys and hows of scientific publishing

Author: Zoe Budrikis[None]

Scientific publishing has changed a lot in recent years, with ever-increasing outputs, new content like code and data, and new algorithm-driven ways of finding information. But even things we take for granted, like abstracts and peer-review, have surprising histories. In this talk I'll share some of that story and give an editor's view on where we are now and what the future might hold.

Field of Condensed Matter:

Magnetism

Superconductivity / **118**

Direct writing of Josephson-like nanojunctions on high-Tc superconductors using a thermal scanning probe

Author: Hanh Duong[1]

Co-authors: Amanuel Berhane [1]; Avi Bendavid ; Emma Mitchell [1]; Simon Lam [1]

[1] *CSIRO*

We demonstrate a direct-write method for creating weak-link Josephson junctions in high-Tc superconducting thin films using thermal scanning probe lithography (t-SPL). A nanoscale heated tip locally modifies the superconductor with sub-10-nm precision, forming constrictions without resists, ion exposure, or multi-step patterning. The resulting nanobridges exhibit Josephson-like characteristics, including non-dissipative supercurrent transport and magnetic-field interference. This single-step thermal patterning approach offers a clean, resist-free fabrication pathway toward scalable quantum devices.

Field of Condensed Matter:

Superconductivity

Magnetism / **119**

Predicting nonreciprocal spin wave generation in magnetic thin films with interfacial DMI

Author: Karen Livesey[1]

[1] *University of Colorado - Colorado Springs & University of Wollongong*

The interfacial Dzyaloshinskii-Moriya Interaction (iDMI) occurs at the surface between a ferromagnet and a heavy metal. In the past 15 years, it has led to interesting magnetic phenomena such as room temperature skyrmions and asymmetric domain wall motion. [1] Spin wave propagation is nonreciprocal when there is iDMI. That is, spin waves of the SAME frequency have different wavelengths when propagating left versus right. This has important applications in creating nonreciprocal microwave devices such as isolators and circulators.

In this talk, I will discuss our recent theoretical work on spin waves with iDMI, in two projects. In the first, I will discuss a weak but previously unknown quadratic dependence of spin wave frequencies on the iDMI strength. [2] Previously, spin wave frequencies were thought to depend linearly on the iDMI strength.

In the second, ways to generate nonreciprocal spin waves will be detailed, using a wire driving a microwave current. We develop a semi-analytic method for predicting the wire width, applied field strength and driving frequency which will maximise the nonreciprocity. [3] The results are confirmed using micromagnetic simulations.

Authors: Rair Macedo, Cameron McEleney, Ellen Lu, Robert Camley, Kristen Buchanan & Karen Livesey

[1] R.E. Camley and K.L. Livesey, *Surf. Sci. Rep.* **78**, 100605 (2023)
[2] E. Lu, K.S. Buchanan and K.L. Livesey, *Phys. Rev. B* **111**, 064432 (2025)
[3] C. McEleney, K.L. Livesey, R.E. Camley and R. Macedo, *submitted* (2026)

Field of Condensed Matter:

Magnetism

Magnetism / **120**

LBMO Nanocrystals for Synergetic Magnetic Hyperthermia Therapy

Author: Alice O'Keefe[1]

Co-authors: Anson Tsan Yin O [1]; Moeava Tehei [1]

[1] *University of Wollongong*

Lanthanum–barium manganite (La(1-x)Ba(x)MnO3, LBMO) nanocrystals were synthesised with barium substitution levels spanning x = 0.1–0.5 in order to systematically probe the influence of compositional doping and calcination temperature on magnetic behaviour relevant to nano-magnetic

hyperthermia applications. Samples were prepared via glycine nitrate solution combustion synthesis process and calcined at 800, 1000, and 1200℃ to explore the interplay between thermal processing, crystallite size, and magnetic phase stability.

Structural and magnetic characterisation revealed a strong dependence of magnetic ordering on both dopant concentration and calcination temperature. At lower calcination temperatures, incomplete crystallisation and suppressed magnetic ordering were observed, while higher temperatures promoted grain growth and the onset of bulk-like ferromagnetic behaviour. Notably, samples with a barium concentration of approximately 10% (x ˜ 0.1), calcined at 1000℃, formed nanocrystalline phases exhibiting superparamagnetic behaviour with a Curie temperature within the biologically relevant range for controlled thermal activation.

This combination of superparamagnetism and tailored Curie temperature is desirable for magnetic hyperthermia, as it enables efficient heat generation under alternating magnetic fields while limiting overheating of surrounding healthy tissue. The results demonstrate that careful tuning of dopant concentration and calcination temperature provides a viable route to engineering LBMO nanocrystals optimised for targeted thermal deposition in brain tumour environments. These findings establish synthesis–structure–property relationships needed to develop a rational design of oxide-based magnetic nanomaterials for biomedical hyperthermia therapies.

Field of Condensed Matter:

Biophysics and medical applications

Quantum science & technology / **121**

Electrostatic Artificial Crystals as a Platform for Correlated Quantum States

Author: Oleh Klochan[None]

Co-authors: Daisy Wang [1]; Zeb Krix [2]; Oleg Sushkov [3]; Alex Hamilton [1]

[1] *UNSW*

[2] *University of Basel*

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The collective electronic properties of solids arise from the interplay of crystal structure and electron–electron interactions. Many of the mechanisms behind these phenomena remain unresolved, motivating the creation of artificial qyuantum simulators that reproduce the essential physics while enabling precise, independent tuning of underlying parameters.
In this work, we demonstrate a fully tunable solid-state artificial crystal formed by imposing a periodic electrostatic potential on a high-mobility 2D electron gas in an ultra-shallow (25 nm) GaAs quantum well. The resulting 100 nm-period triangular lattice establishes a new, electrically controllable bandstructure distinct from the host crystal. Transport signatures directly reveal this engineered bandstructure. Uniquely, our electrostatic approach enables continuous tuning between qualitatively different dispersions: graphene-like linear bands and kagome-like bands within a single device.

At half filling of the kagome flat band, we observe a pronounced insulating state inconsistent with a single-particle picture. Its characteristics are consistent with a loop-current Wigner insulator, a correlated electronic phase driven by long-range Coulomb interactions and electron delocalisation between neighbouring empty sites—behaviour unique to kagome geometries.

Our results establish a new, versatile platform where lattice geometry, band flatness, and interaction strength can be continuously tuned in situ. This provides a powerful route for exploring correlated quantum phases and engineering designer electronic materials in a reproducible and highly controllable semiconductor environment.

Field of Condensed Matter:

Quantum Materials

Superconductivity / **122**

High laser fluence: the new strategy for depositing High Temperature Superconducting films for applications

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The established guiding principle for pulsed laser deposition (PLD) of high-quality $YBa_2Cu_3O_{7-x}$ (YBCO) superconducting films suggests that the optimal target-to-substrate distance (TSD) lies near the visible tip of the laser-induced plume, with deviations from this point expected to degrade film properties. We modified our PLD system to allow precise external TSD adjustment over a 110 mm range and systematically studied its influence on the electromagnetic, micro- and nanostructural properties of YBCO thin films. Our analysis, referencing plume propagation models and growth processes, reveals that the optimal TSD range can, in fact, be extended under relatively high laser fluence, depending on the desired film performance and properties. We identify four TSD regimes, each exhibiting unique film characteristics. X-ray diffraction (XRD) θ–2θ scans reveal lattice parameter splitting at the 001 and 002 reflections through the formation of triple peaks, indicative of a tri-layered strain structure. This is the first report of such a structure under nominally monolayer growth conditions without additional fabrication techniques, spanning a 50 mm TSD range. The phenomenon arises from the combined influence of TSD and laser fluence, driving transitions between monolayer and multilayer-like growth. Remarkably, high-quality superconducting properties and crystallinity are preserved across a broad 50 mm TSD window, yielding films with variable total thickness, layer thickness, surface structure, and growth modes. This insight and tunability deepen understanding of growth mechanisms and deposition dynamics, offering new pathways to tailor surface morphology and performance in electronics and high-power applications through controlled structural evolution and efficient deposition rates.

Field of Condensed Matter:

Superconductivity

Topological materials / **123**

Artificial Quantum Matter

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Artificial crystals, formed by imposing spatially periodic potentials onto existing material platforms, provide a powerful route for designing and controlling electronic properties beyond those available in natural systems. Moiré superlattices in twisted two-dimensional (2D) materials have recently emerged as a prominent example, hosting correlated insulating states, superconductivity, and other strongly interacting quantum phases in graphene-based systems. However, moiré lattices are fundamentally constrained by the symmetry of the underlying 2D crystals and the twist angle between layers, which can introduce non-uniform long-range strain and limit lattice uniformity. In addition, the strength of the modulation potential is largely fixed once the device is fabricated, restricting

post-fabrication tunability.
To overcome these limitations related to strain and device flexibility, we present an alternative and highly tuneable approach to artificial quantum matter based on imposing spatially periodic electric potentials using patterned metallic gate architectures. Such gate-defined superlattices enable the realization of artificial crystals with arbitrary lattice symmetries, tuneable lattice constants, and controllable modulation strengths, while remaining compatible with a wide range of material platforms, including conventional semiconductors and van der Waals heterostructures.
We fabricate these devices through a sequence of advanced nanofabrication steps, ranging from mechanical exfoliation of high-quality flakes to full device assembly and packaging. To enhance electron mobility in the transport channel and reduce contact resistance, optimized forming-gas annealing and precisely controlled reactive ion etching processes are employed. Finally, using magnetotransport and radio-frequency capacitive measurements at ultralow temperatures, we investigate emergent quantum phases arising from engineered band topology, electron–electron interactions, and magnetic-field-induced effects.

Field of Condensed Matter:

Topological Materials

Topological materials / 129

Stability and Conductivity of Ferroelectric Nanoscale Bubbles toward Low-Energy Electronic Devices

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Nanoscale ferroelectric topologies such as vortices, skyrmions, and bubble domains are stabilized in thin films through a delicate balance of mechanical and electrical boundary conditions. In particular, sub-10 nm ferroelectric bubbles promise intriguing functional properties for next-generation solid-state electronic devices[1-2]. However, a systematic understanding of their phase stability and dynamic conductivity remains elusive.
Here, we address this gap using first-principle-based simulations and scanning probe microscopy on ultrathin epitaxial (001) $PbZr_{0.4}Ti_{0.6}O_3$ heterostructures. Simulations predict that labyrinthine domains transform into bubbles under reduced film thickness, increased mechanical pressure, and/or improved electrical screening. This transition is driven by a mechanism that conserves the residual depolarization field, pinned by an external or built-in electric bias. These predictions are experimentally verified using tomographic atomic force microscopy, demonstrating controlled manipulation of nanoscale bubble domains through concurrent effect of reducing film thickness and increased mechanical stimulus[3].
In addition, we investigate the conduction properties of as-grown bubbles in PbZr0.2Ti0.8O3 heterostructures. At bubble sites, rectifying current-voltage characteristics with ultra-high current densities have been observed, attributed to tunneling. Conductivity is maintained or enhanced under an external electric field, provided the bubble configuration remains stable. Conversely, mechanical disruption of the dipolar configuration decreases conductivity by 50%. Simulations highlight the role of inhomogeneous depolarizing fields and screening conditions in dynamically tuning tunneling transport.
Our findings provide a comprehensive understanding of the phase stability and dynamic conductivity of ferroelectric bubbles, offering new opportunities for their application in future electronic and functional devices.

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Field of Condensed Matter:

Energy and Functional Materials

Nanoparticles / **131**

Radiation as a Sculptor

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The synthesis of radioactive gold nanoparticles (^{198}AuNPs) for nuclear medicine traditionally involves complex, multi-step procedures requiring the handling of highly radioactive bulk materials, dissolution in harsh acids, and the use of toxic chemical reducing agents. This work explores a "one-pot" radiolytic synthesis method that exploits the dual nature of neutron irradiation to simultaneously activate the gold and drive nanoparticle synthesis.

The process relies on the Szilárd-Chalmers effect, where the recoil energy imparted by prompt gamma emission following neutron capture ($^{197}\mathrm{Au}(n,\gamma)^{198}\mathrm{Au}$) breaks the metallic lattice bonds. This physical recoil ejects radioactive ^{198}Au atoms directly into the surrounding aqueous medium, primarily as $^{198}\mathrm{Au}^{3+}$ ions.[1] Experiments demonstrate that foils irradiated in water yield an order of magnitude higher radioactivity in the liquid phase compared to foils irradiated dry, confirming the efficacy of this recoil-mediated ejection mechanism.

Once ejected, the gold ions undergo reduction driven by the radiolysis of the aqueous solvent. The gold-water interface creates a unique radiochemical environment; the high atomic number of gold ($Z = 79$) leads to a massive release of secondary Auger electrons, resulting in a nanoscopic dose enhancement of 400–600 times in the interfacial water layers.[2] This localized energy deposition amplifies the production of hydrated electrons (e^-_{aq}), which act as potent reducing agents, converting the ejected Au^{3+} into zero-valent Au^0 and initiating nucleation. This method allows for the production of sterile, surfactant-free radioactive nanoparticles suitable for nanobrachytherapy without the need for external chemical reducers.[3]

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Field of Condensed Matter:

Biophysics and medical applications

Materials and devices / **132**

Simultaneous study of acoustic and optic phonon scattering of electrons and holes in undoped GaAs/AlGaAs heterostructures

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The study of phonon coupling in doped semiconductors via electrical transport measurements is challenging due to unwanted temperature-induced effects such as dopant ionization and parallel conduction. Here, we study phonon scattering in 2D electrons and holes in the 1.6–92.5 K range without the use of extrinsic doping, where both acoustic and longitudinal optic (LO) phonons come into effect. We use undoped GaAs/ AlxGa1–xAs heterostructures and examine the temperature dependence of the sample resistivity, extracting phonon coupling constants and the LO activation energy. Our results are consistent with results obtained through approaches other than transport measurements and highlight the benefit of this approach for studying electron–phonon and hole–phonon coupling.

Field of Condensed Matter:

Quantum Materials

Magnetism / **133**

Electronic scattering of Weyl electrons off magnetic hopfions

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Magnetic hopfions are three-dimensional topological spin textures characterised by non-local invariants and a rich internal structure, making them promising candidates for novel spintronic and transport phenomena. Weyl semimetals provide a natural electronic platform to probe such textures, as their low-energy quasiparticles behave as relativistic chiral fermions that are highly sensitive to magnetic order.
In this work, we investigate the scattering of Weyl electrons from magnetic hopfions. We model the coupling between the electron spin and the local magnetisation through an exchange interaction and analyse the resulting scattering problem using both the Born and eikonal approximations, highlighting the distinct physical regimes in which each approach applies. Our results demonstrate how the internal structure of hopfions imprint characteristic signatures on Weyl electron scattering as compared to that of conventional electrons with quadratic dispersion relations. This provides a potential route for scattering signatures to be detected in magnetic Weyl semimetals.

Field of Condensed Matter:

Magnetism

Topological materials / **135**

Artificially synthesised topological insulators in engineered semiconductor nanostructures

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In this work we investigate an approach [1] to artificially synthesise a band-inverted topological insulator (TI) using a superlattice (SL) in InAs/GaInSb semiconductor material system. In particular, we explore the possibilities of creating a TI with a flat-band quasiparticle spectrum for realising new emergent superconductivity physics, either in the form of the unconventional bulk superconductivity [2] or by interfacing the TI with a conventional superconductor.
Theoretical modelling of the E(k_x, k_y, k_z) band structure is performed using 8-band $k \cdot p$ method to determine the design parameters of InAs/GaInSb SLs, corresponding to the material phases of conventional semiconductor, zero-gap semimetal, and inverted-band topological insulator. We also obtain the constant energy surfaces at different levels of chemical potentials (Fermi energy) and evaluate expected topological states that can be created in these material phases.
The TI candidate structure is based on InAs/GaInSb SL with an engineered bulk energy gap of 15-20 meV. It has been fabricated by molecular beam epitaxy (MBE) on GaSb(100) substrate. This growth technique can preserve the rotational symmetries of the crystal lattice along the growth direction and ensure that the topological states existing between the TI bulk material and interfacial layers or vacuum are topologically protected.
We also report on magnetoresistance (R_{xx}) and Hall resistance (R_{xy}) measurements of this structure, demonstrating metallic-like temperature dependence of the resistivity below T<30K, non-saturating R_{xx}, and Shubnikov–de Haas magneto-oscillations of multiple quasiparticle species attributed to the bulk and surface states.

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Field of Condensed Matter:

Quantum Materials

Magnetism / 136

Linear spin wave analysis of the Kitaev spin liquid candidate Li_3 Co_2 SbO_6

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The search for a quantum spin liquid (QSL) has stimulated substantial research activity within condensed matter physics, particularly following Kitaev's proposal of his paradigmatic exactly solvable

spin model. This model hosts a true QSL ground state and provides an elegant framework for fractionalisation, in which the original spin degrees of freedom decompose into emergent quasiparticles comprising static $\mathbb{Z}_2$ gauge fluxes (visons) and itinerant Majorana fermions. Despite its profound implications for topological quantum computing, a material realisation of the pure Kitaev model has not yet been achieved. This limitation primarily arises from the presence of additional conventional spin interactions, such as Heisenberg and anisotropic Γ exchanges, which compete with the Kitaev term and prevent the system from forming a true QSL state. Nevertheless, depending on the relative strength of the Kitaev interaction, candidate materials may in principle be tuned into a QSL phase through external perturbations such as applied magnetic fields or lattice strain. More recently, cobalt-based quantum magnets have been identified as promising platforms for realising the bond-dependent Kitaev interactions central to this model. One such candidate material, $Li_3Co_2SbO_6$, has been reported to exhibit an A-type antiferromagnetic order. By using inelastic neutron scattering (INS) and linear spin wave theory (LSWT), we have phenomenologically extracted the effective coupling parameters of an extended Kitaev–Heisenberg spin model for this compound. The comparatively strong Kitaev exchange inferred from this analysis places $Li_3Co_2SbO_6$ as a promising Kitaev spin liquid candidate, despite having an A-type antiferromagnetic ground state. This is in contrast with its sister compound $Na_3Co_2SbO_6$, which stabilises a zigzag antiferromagnetic ground state.

Field of Condensed Matter:

Magnetism