CMQM 2023

Condensed Matter and Quantum Materials

28–30 June 2023

University of Birmingham, Birmingham, UK

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Condensed Matter and Quantum Materials (CMQM 2023)

Programme

Wednesday 28 June 2023
Bramwell Foyer, Bramwell Music Building

5pm – 7pm	Registration and Drinks Reception

Thursday 29 June 2023
The Teaching and Learning Building

8:15am - 9am	Registration and Arrival Refreshments
9am - 9:30am	**Plenary Session 1. Room: Theatre 1 (Upper Ground Floor)** **David Cobden:** Topology, superconductivity, excitons and ferroelectricity all in one place
9:30am - 10:30am	**Magnetism 1. Room: Theatre 1 (Upper Ground Floor)** **Joseph Barker** (9:30am-10am): Calculating thermodynamics, magnons and spin currents in complex magnetic materials using atomistic spin dynamics **Stephen Blundell** (10am-10:15am): The quantum muon as a probe of magnetic frustration **Dr. Manuel Dos Santos Dias** (10:15am-10:30am): Topological magnons driven by the Dzyaloshinskii-Moriya interaction in the centrosymmetric ferromagnet Mn5Ge3
	Superconductivity 1. Room: Theatre 2 (First Floor) **Dr Jake Ayres** (9:30am-10am): Magnetotransport and Dual Character of Cuprates **Wangping Ren** (10am-10:15am): On the Electron Pairing Mechanism of Copper-Oxide High Temperature Superconductivity **Charles Tam** (10:15am10:30am): Two component charge fluctuations in La2-xSrxCuO4
	Metals and Correlated Electron Systems 1. Room: 118/119 (First Floor) **Dr Andreas W. Rost** (9:30am-10am): Entropy of Quantum Materials **Shiyu Deng** (10am-10:15am): Dynamics of the critical phonon modes in quantum paraelectric $SrTiO_3$ **Mr Jacopo Radaelli** (10:15am-10:30am): Plasmons in a bilayer cuprate
	Semiconductors. Room: 109 (First Floor) **Dr Taylor Stock** (9:30am-10am): High-yield atomically precise fabrication using arsenic in silicon and germanium **Chak Lam Chan** (10am-10:15am): Site-controlled InAs/GaAs Quantum Dot arrays for nanophotonics **Patrick Williams** (10:15am-10:30am): An ab initio Study of Electron Transport in Ultra-Wide Band Gap Semiconductors
10:30am - 11am	Morning Break Sponsored by Oxford Instruments Nanoscience
11:00am - 1pm	**Helium and Complex Structured Materials. Room: Theatre 1 (Upper Ground Floor)** **Professor Neil Wilson** (11am-11:30am): Electronic structure measurements of 2D materials, with a twist **Fabrizio Cossu** (11:30am-11:45am): Structural and magnetic competition in (111)-oriented manganite superlattices **Dr Petri Heikkinen** (11:45am-12pm): Topological superfluid helium-3 under mesoscopic confinement **Dr Oleg Kirichek** (12pm-12:15pm): 4He and 3He – 4He mixture films studied by neutron reflectometry **Tineke Salmon** (12:15pm-12:30pm): QUEST-DMC: Superfluid Helium-3 Bolometers for a Direct Dark Matter Search **Liam Turnpenny** (12:30pm-12:45pm): Phase transition and Moiré superlattices in the two-dimensional single and few-layer NiI2 transition metal dihalide

11:00am - 1pm	**Superconductivity 2. Room: Theatre 2 (First Floor)** **Bernd Braunecker** (11am-11:15am): Supercurrent-enabled Andreev reflection in a chiral quantum Hall edge state **Amalia Coldea** (11:15am-11:30am): Fermi surfaces and quasiparticle effective masses in the high-pressure phase of superconducting iron-chalcogenides, FeSe1-xSx **Emily Gamblen** (11:30am-11:45am): Probing the superconducting transition in 2D materials with graphene-based SQUIDs **Archie Morfoot** (11:45am-12pm): Anisotropic band splitting induced by applied strain to a tetragonal FeSe1-xSx **Searbhán Ó Peatáin** (12pm-12:15pm): Characterization of Titanium-Nitride Thin Films & Design of Kinetic Inductance Travelling Wave Parametric Amplifier **Emil Rizvanov** (12:15pm-12:30pm): Numerical simulation of Josephson traveling-wave parametric amplifier **Rais Shaikhaidarov** (12:30pm-12:45pm): Current quantization due to the a.c. coherent quantum phase slip effect **Mr Max Taylor** (12:45pm-1pm): Fractional Shapiro steps in graphene SQUIDs
	Metals and Correlated Electron Systems 2. Room: 118/119 (First Floor) **Dr Silvia Ramos** (11am-11:30am): Structural signatures of metal-insulator transitions as seen by polarisation dependent x-ray absorption spectroscopy **Carolina De Almeida Marques** (11:30am-12pm): Enhanced surface magnetism in the ferromagnetic Sr4Ru3O10 **Prof Andrew Green** (12pm-12:30pm): The Role of Quantum Computation in Condensed Matter Physics **Michal Moravec** (12:30pm-12:45pm): Directional Ballistics in Ultra-Pure Delafossite Metals **Thomas Sheerin** (12:45pm-1pm): Non-Fermi Liquid Behaviour Induced by Gauge-Field Interactions: Insights from the Functional Renormalization Group
	Topological Materials 1. Room: 109 (First Floor) **Dirk Backes** (11am-11:15am): Evaluating and optimising proximity-induced magnetism in MnTe/Bi2Te3 heterostructures **Gabriel Cardoso** (11:15am-11:30am): Exact Results on the Anomalous Hall Effect in the Dirac Semimetal ZrTe5 **Dr Malcolm Connolly** (11:30am-11:45am): Integration of semiconductor Josephson junctions in superconducting quantum circuits **Dylan Jones** (11:45am-12pm): Flat bands, localised states, and non-trivial topology of one-dimensional Lieb superlattices **Philipp Kagerer** (12pm-12:15pm): The 2D Ferromagnetic Extension of a Topological Insulator
1pm - 2:50pm	**Lunch, Poster Session and Exhibition**
2:50pm - 3pm	**Presentation by Cryogenic. Rooms: Theatre 1 (Upper Ground Floor) and Theatre 2 (First Floor)**
3pm - 5:30pm	**Vinen Memorial Session. Room: Theatre 1 (Upper Ground Floor)** **Dr Chris Muirhead** (3pm-3:30pm): W.F. (Joe) Vinen: a brief summary of Joe's career and his many achievements **Prof Carlo Barenghi** (3:30pm-4pm): Quantum turbulence - the scientific legacy of W. F. Vinen **Professor Peter McClintock** (4pm-4:30pm): Using negative ions to measure Joe Vinen's energy barrier **JC Seamus Davis** (4:30-5pm): Quantization of Macroscopic Phenomena **Professor Ladislav Skrbek** (5pm-5:30pm): Collective dynamics of ions and vortices in He II in experiments of Joe Vinen
	M4QN Focus Session. Room: Theatre 2 (First Floor) **Thorsten Hesjedal** (3pm-3:30pm): Bringing Magnetic Order to Topological Insulators **Martin Weides** (3:30pm-4pm): Optimizing Materials in Superconducting Quantum Circuits **Dr Otto Mustonen** (4pm-4:30pm): Spin-liquid-like states in perovskite-related phases **Professor Geetha Balakrishnan** (4:30pm-5pm): Investigations of Skyrmion materials **Dr Sanjeev Kumar** (5pm-5:30pm): Fractional conductance in one-dimensional electrons
5:40pm - 6:15pm	**Evening Talk. Room: Theatre 1 (Upper Ground Floor)** Professor Carl Chinn, historian of the city of Birmingham: Talk: Making of the Modern World
6:30pm - 10:30pm	**Conference Drinks Reception and Dinner** Botanical Gardens, Westbourne Road, Birmingham, B15 3TR A bus will be operating between the University and the venue and the return journey

Friday 30 June 2023
Teaching and Learning Building

8:30am – 9am	Arrival Refreshments
9am - 9:30am	**Plenary Session 2. Room: Theatre 1 (Upper Ground Floor)** **Peter Littlewood**: Materials for energy and sustainability
9:30am-10:30am	**Magnetism 2. Room: Theatre 1 (Upper Ground Floor)** **Dr Matthew Coak** (9:30am-10am): Tuning dimensionality, magnetism and conduction in van-der-Waals Mott insulators TMPS3 **Marios Georgiou** (10am-10:15am): Multi-Q magnetic phases from frustration and chiral interactions **Jack Harrison** (10:15am-10:30am): Flexure-induced strain control of antiferromagnetic domains in crystal membranes
	Atomic, Molecular and Optical Physics. Room: Theatre 2 (First Floor) **Dr Charles Creffield** (9:30am-9:45am): Correlated superfluidity produced by Floquet driving **Angus Crookes** (9:45am-10am): Strong Coupling and Entanglement in Extreme Nanophotonic Cavities **Takla Nateeboon** (10am-10:15am): Effects of cavity and atomic decay rates on efficiencies of quantum memory **Dr Hannah Stern** (10:15am-10:30am): Coherent Control of a Single Electronic Spin in a 2D Material at Room Temperature
	Facilities 1. Room: 118/119 (First Floor) **Cephise Cacho** (9:30am-10am): Photon-based characterisations of Quantum Material at Diamond Light Source **Pascal Manuel** (10am-10:30am): New opportunities for Quantum materials research at the ISIS neutron and muon source
	Metals and Correlated Electron Systems 3. Room: 109 (First Floor) **Petra Grozić** (9:30am-9:45am): Magnetocondoctivity of CaC6 with a CDW-reconstructed Fermi surface **Larissa Ishibe Veiga** (9:45am-10am): The 3d-5d exchange interactions and orbital hybridization in Ba- and Ca-doped La2CoIrO6 double perovskite **Barbara Keran** (10am-10:15am): DC Transport and Magnetotransport Properties of the 2D Isotropic Metallic System with the Fermi Surface Reconstructed by the Charge Density Wave **Alex Louat** (10:15am-10:30am): Termination-dependent surface states and bulk band structure of LaTe2
10:30am – 11am	Morning Break Sponsored by Oxford Instruments Nanoscience
11am – 1pm	**Magnetism 3. Room: Theatre 1 (Upper Ground Floor)** **Dr Jennifer Fowlie** (11am-11:30am): Intrinsic magnetism in superconducting nickelate heterostructures **Dr Berit Goodge** (11:30am-12pm): Solving the polar interface in superconducting nickelate thin films **Dr Daniel Mayoh** (12pm-12:15pm): Magnetic properties of the intercalated transition metal dichalcogenide Fe1/3TaS2 **Dr Thomas Moore** (12:15pm-12:30pm): Separation of heating and magneto-elastic coupling effects in surface acoustic wave-enhanced magnetic domain wall creep motion **Dr Thomas Nussle** (12:30pm-12:45pm): Numerical simulations of spin dynamics using a path integral method **Wei Peng** (12:45pm-1pm): Electron skew scattering by ferroelastically frustrated magnetic spins
	Topological Materials 2. Room: Theatre 2 (First Floor) **Dr Bartomeu Monserrat** (11am-11:30am): From single to multi-gap topological materials **Sian Dutton** (11:30am-12pm): Magnetism on the stretched diamond lattice in lanthanide orthotantalates **M. M. McCarthy** (12pm-12:15pm): A topological classification of finite chiral structures – theory and experiment **Songyang Pu** (12:15pm-12:30pm): Signatures of Supersymmetry in the v=5/2 Fractional Quantum Hall Effect **Professor D.M. Whittaker** (12:30pm-12:45pm): Topological Physics in Coaxial Cable Networks **Dr Wei Wu** (12:45pm-1pm): Topological properties of a one-dimensional excitonic model combining local excitation and charge transfer

11am – 1pm	**Facilities 2. Room: 118/119 (First Floor)** **Professor Amalia Patanè** (11am-11:15am): Science and Technologies at the European Magnetic Field Laboratory **Sean Collins** (11:15am-11:30am): Probing the heterogeneity of electronic structure at the nano- to atomic-scale at SuperSTEM **Professor Roger Webb** (11:30am-11:45am): Ion Implantation for Solid State Quantum Technologies **Dr Yvonne Grunder** (11:45am-12pm): XMaS: The UK Materials Science Facility at the ESRF **Dr David Cox** (12pm-12:15pm): Deterministic Single Ion Implantation at the NIBC and the RAISIN Network **Dr Edmund Clarke** (12:15pm-12:30pm): EPSRC National Epitaxy Facility enabling semiconductor research in the UK **Dr Dinu Iuga** (12:30pm-12:45pm): High-Field Solid-State Nuclear Magnetic Resonance National Research Facility **Dr Mark Isaacs** (12:45pm-1pm): HarwellXPS – The UK National Facility for XPS; Analysis and Advances
	Surfaces, Interfaces and Thin Films. Room: 109 (First Floor) **Akhil Rajan** (11am-11:30am): Surfactant-mediated epitaxial growth of large-area transition-metal dichalcogenides **Assoc Prof Robert Edward** (11:30am-11:45am): Antimony trisulfide: from local structural transitions to programmable photonics **Edward Dunn** (11:45am12pm): Ambient characterisation of atomic defects in transition metal dichalcogenides with single atom resolution **Chris Hooley** (12pm-12:15pm): Hierarchy of Lifshitz transitions in the surface electronic structure of Sr2RuO4 under uniaxial compression **Dr Juliana Morbec** (12:15pm-12:30pm): Designing organic/2D heterostructures for photovoltaic applications **Dr Rebecca Nicholls** (12:30pm-12:45pm): Structure and Phase Transformations of Metastable Hexagonal Uranium Thin Films **Alessio Quadrelli** (12:45pm-1pm): Activation of 2D polymerisation on inert surfaces with atomic clusters as extrinsic catalysts
1pm – 3pm	Lunch, Poster Session and Exhibition
3pm – 5pm	**Magnetism 4. Room: Theatre 1 (Upper Ground Floor)** **Dr Sam Ladak** (3pm-3:30pm): Magnetic Charge Ordering in 3D Artificial Spin-ice **Ioannis Rousochatzakis** (3:30pm-4pm): The role of symmetric off-diagonal exchange in Kitaev honeycomb antiferromagnets **Shroya Vaidya** (4pm-4:15pm): Magnetic Ground States of Non-linear Antiferromagnetic Coordination Polymer Chains **Ieuan Wilkes** (4:15pm-4:30pm): Materials Optimisation for Next Generation Low Power Electronic Devices **George Wood** (4:30pm-4:45pm): The Double-Q Ground State with Topological Charge Stripes in the Centrosymmetric Skyrmion Candidate GdRu2Si2 **Xiaotian Zhang** (4:45pm-5pm): Magnetoelectric coupling of Terbium Tantalate
	Superconductivity 3. Room: Theatre 2 (First Floor) **Professor Andrew Huxley** (3pm-3:30pm) **Dr Sven Friedemann** (3:30 PM - 4:00 PM): High-Magnetic-Field Studies of Hydride High-Temperature Superconductors **James Annett** (4:00 PM - 4:15 PM): Modelling strain experiments in unconventional superconductors **Weijiong Chen** (4:15 PM - 4:30 PM): Interplay of Hidden Orbital Order and Superconductivity in CeCoIn5 **Morgan Grant** (4:30 PM - 4:45 PM): Magnetic penetration depth measurements of the superconducting energy gap structure of UTe2 **Lev Levitin** (4:45 PM - 5:00 PM): Unconventional superconductivity underpinned by antiferromagnetism in $YbRh_2Si_2$
	Metals and Correlated Electron Systems 4. Room: 118/119 (First Floor) **Dr Cameron Dashwood** (3pm-3:30pm): Strain control of a bandwidth-driven spin reorientation in Ca3Ru2O7 **Professor Joseph Betouras** (3:30pm-4pm): Higher order van Hove singularities in quantum materials **Anirudh Chandrasekaran** (4pm-4:15pm): Possible role of higher order singularities in Sr2RuO4 – a theoretical perspective **Dr Luke Rhodes** (4:15pm-4:30pm): Stabilization of in-plane ferromagnetism at the surface of quantum critical Sr3Ru2O7

3pm – 5pm	**1. Nonequilibrium Physics 2. Instruments and Applications. Room: 109 (First Floor)** **Zhengming Wu** (3pm-3:15pm): NanoFrazor Lithography for advanced 2D&3D nanodevices **Dr Jan Nyeki** (3:15pm-3:30pm): High performance rapid turn-around cryogen-free microkelvin platform: unlocking the sub-1mK temperature range for quantum materials research **Dr. Charles Downing** (3:30pm-3:45pm): Exceptional points from two-photon driving **George McArdle** (3:45pm-4:00pm): Absence of thermalisation in a quantum dot **Dr Jessica Boland** (4pm-4:30pm): SNOM lights up the nanoscale: non-destructive nanoscale optoelectronic characterisation via scattering-type Near-field optical microscopy **Jonathan Alaria** (4:30pm-4:45pm): Chemically controllable magnetic transition temperature and magneto-caloric properties in MnZnSb based compounds **Dr Joseph Prentice** (4:45pm-5pm): Efficient computation of optical properties of large-scale heterogeneous systems
5pm – 5:10pm	Depart

Poster Presentions

Poster Number	Name	Paper Title
1	Aisha Albeladi	Unlocking the Hidden Power: Unravelling Sub-Bandgap Photoconductivity in Synthetic Cu2O under Pulsed Laser Excitation at IR wavelength
2	Rasha Algethami	Modelling of Microstructure Evolution During Polymer Crystallisation
3	Hanan Alhabeadi	Statistical Analysis of the Distribution of single atoms and Nanoclusters on Surfaces
4	Dr Abhisek Bandyopadhyay	Sr3LiIrO6: a potential quantum spin liquid candidate in quasi-1-D d4 iridate family
5	Dr Deepnarayan Biswas	Soft X-ray angle-resolved photoelectron spectroscopy with a momentum microscope at Diamond Light Source
6	Chandan Singh	Superconductor/ferromagnet van der Waals heterostructure: Appearance of Majorana zero mode
7	Amit Chauhan	Exploration of novel quantum phases and large magnetic anisotropy energy in low-spin d5 perovskites: Bulk and Ultra-thin films
8	Dr Matthew Coak	SquidLab - a user-friendly program for background subtraction and fitting of magnetization data
9	Dr Arthur Coveney	Rapid Prototyping of Novel Devices with In-situ Deposition, Imaging and Thermal Nanolithography
10	Sam Cross	Superconductivity at 90 K in a lanthanum hydride film synthesised using elemental lanthanum and ammonia borane at 95 GPa
11	Deepanjan Das	Exploring quantum paraelectricity as a mechanism for parametric amplification
12	Buddhadeb Debnath	Signatures of Orbital Selective Mott state in doped Sr3Ru2O7
13	Dr Dirk Honecker	Probing the Magnetization Distribution in Ferrite Nanoparticles with Magnetic SANS
14	Aidan Horne	High Resolution Imaging of Silicon Vacancy Colour Centres in Diamond Using 4D-STEM and Electron Ptychography
15	Tim Huijbregts	Suppressing superconductivity in high-Tc cuprates with intense current pulses
16	Clio Johnson	Homogeneous, Isotropic, Three-body Backflow Correlation in Quantum Monte Carlo Simulations
17	Saba Khan	Vibrating carbon nanotubes: A nanomechanical probe to study quantum phenomena in superfluid 3He/4He
18	Colin Kirkbride	Fullerene Thin Films as a Route to Skyrmion Nucleation
19	Hemant KumarLimbu	Molecular dynamics study on the relation between atomic structure and temperature of Mg-Zn alloys for metal air batteries electrodes
20	Elie Merhej	Dynamical correlations in the Hubbard ladder after a pump-probe quantum quench
21	Sang Soon Oh	Euler class for topological phase transition of nodal lines in spring-mass systems
22	Ioana Paulescu	Quantum oscillations of a candidate bulk Dirac system
23	David Reid	Theoretical investigation on topologically robust edge-states in a harmonic synthetic dimension and its experimental realisation.
24	Professor John Saunders	Quantum bath suppression in a superconducting circuit by immersion cooling
25	Shobhna Singh	THE O(N) LOOP MODEL ON QUASICRYSTALS
26	Dr Hideo Takeuchi	Free induction decay processes of folded longitudinal acoustic phonons dependent on a constituent layer ratio in one period of GaAs/AlAs superlattices in a finite system: Effects of the phonon dispersion curve
27	Amie Troath	Exploring topological excitations of S=1/2 kagome ferromagnets using inelastic neutron scattering
28	Dr Matthew Watson	Novel electronic structures from near-surface stacking faults
29	Huseyin Bilge Yagci	Enhanced collection efficiency from single colour centres in aluminium nitride micropillars
30	Mihir Date	Bulk and surface electronic structure of Nb3Br8

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Sample in vacuum or exchange gas
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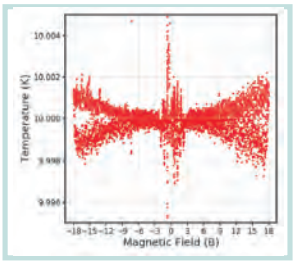

Modulus field along axis with 2.6 T central field

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Resistivity measurements for up 700 K
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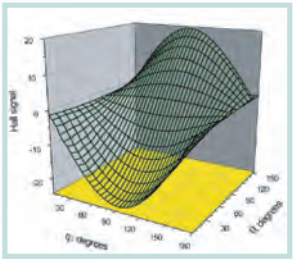
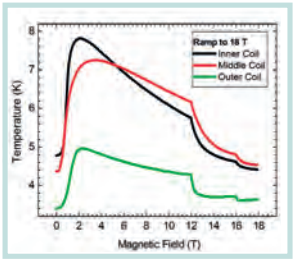


Hall Voltage as a function of polar angle in magnetic field



Ramp of magnetic field to 18 T

High Field Cryogen-Free Magnetic Resonance (MR) Magnets

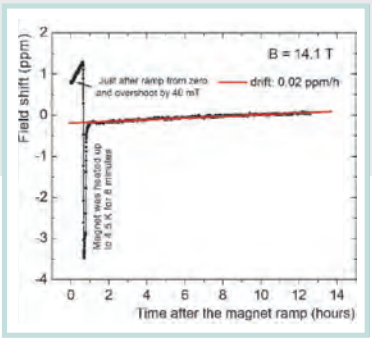
600 MHz cryogen-free NMR magnet system

Cryostat: Cryogen-Free

Completely cryogen-free
Pulse Tube cryocooler
Very low vibration

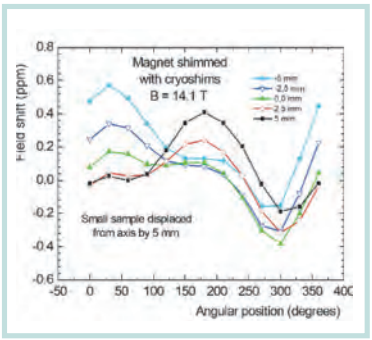
Applications

- NMR
- EPR / ESR
- DNP



Magnet: Fixed and Variable field operation

Operating fields to 16.44 / 700 MHz
≤ 1 ppm fixed field central homogeneity
~ 10 ppm bare field homogeneity in 10 mm DSV
~ 1 ppm field homogeneity with cryoshims
Rapid <<0.1 ppm / hr drift in persistent mode



Sample environment

Room temperature bore: 89 mm / 54 mm
Variable sample temperatures 1.3 K to 400 K

Unit 6 Acton Park, The Vale, London W3 7QE, United Kingdom
Tel: +44 20 8743 6049 **Email:** sales@cryogenic.co.uk

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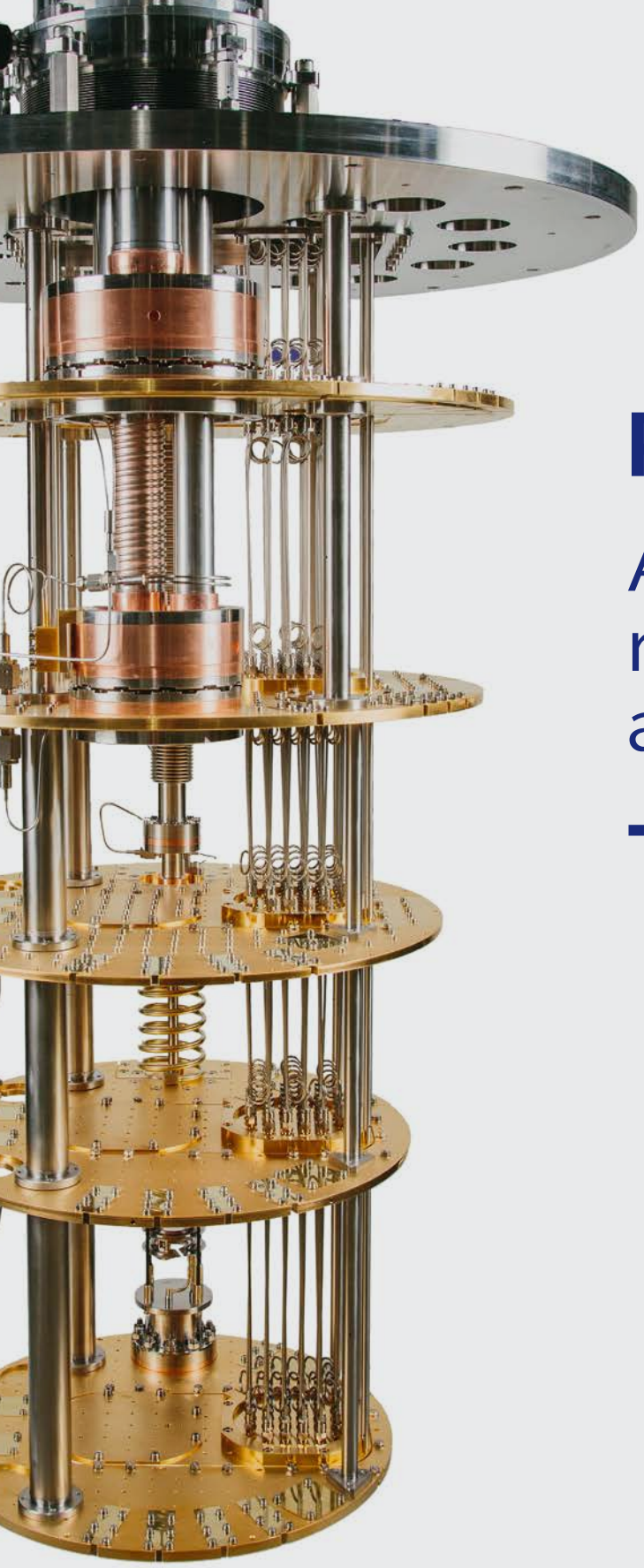

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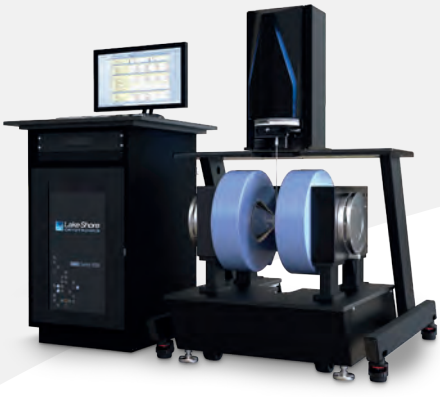

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Invited Speakers

Magnetotransport and Dual Character of Cuprates

Dr Jake Ayres
University of Bristol, United Kingdom

Superconductivity 1, June 29, 2023, 09:30 - 10:30

Understanding the normal state of cuprate superconductors is surely crucial to an understanding of the superconducting state that emerges at lower, but still anomalously high, temperatures. I will summarize recent studies [1, 2] of the in-plane magnetoresistance in which a universal phenomenology of the magnetoresistance has been revealed across multiple families of cuprates. Distinct doping regimes are found to be characterised by distinct scaling behaviours [2]. It is argued that an explanation for the scaling and the universality of the behaviour is beyond any known form of Boltzmann transport. Finally, I will attempt to justify the need for two distinct components to the conductivity and explain the possible relevance of this dual character to the superconducting state [3].

[1] Ayres et al., Nature 595, 661-666 (2021)
[2] Berben et al., arXiv:2203.04867 (2022)
[3] Ayres et al., Front. Phys. 10:1021462 (2022)

Quantum turbulence - the scientific legacy of W. F. Vinen

Prof Carlo Barenghi
Newcastle University, United Kingdom

Vinen Memorial Session, June 29, 2023, 15:00 - 17:30

Vinen's pioneering experiments on heat currents in superfluid helium in the late 1950's were originally aimed at better understanding helium's unusual heat-transfer properties. Vinen's experiments revealed that, at sufficiently large heat flux, the heat transfer is limited by a tangle of quantised vortex lines - a form of turbulence constrained by the quantum mechanical quantization of the circulation. In the 1990's, it became clear that, in some regimes, this quantum turbulence shares important properties with ordinary (classical) turbulence. In other regimes, however, the analogy with classical turbulence fails. Advances in atomic physics led to the study of quantum turbulence in other quantum fluids besides helium 3 and helium 4, such as Bose-Einstein-condensed atomic gases; the possibility of quantum turbulence in astrophysical systems (e.g. neutron stars, cold dark matter) has also been raised. In this talk I shall briefly identify the main types of quantum turbulence which have been experimentally and computationally observed, highlighting analogies and differences with classical turbulence. The aim is to make apparent that Vinen's original investigation has developed into a rich new area of interdisciplinary physics research.

Photon-based characterisations of Quantum Material at Diamond Light Source

Cephise Cacho[1], Alex Louat, Matthew Watson, Timur Kim
[1]*Diamond Light Source, Didcot, United Kingdom*

Facilities 1, June 30, 2023, 09:30 - 10:30

Diamond Light Source is the national UK low energy synchrotron offering to the scientific community 33 operational beamlines in a wide range of techniques. In this presentation I will give an introduction to the experiments frequently performed on Quantum Material e.g. Angle-Resolved Photoemission Spectroscopy (ARPES), Hard X-ray Photoemission Spectroscopy (HAXPES), Surface X-ray Diffraction (SXRD), Resonant Inelastic X-ray Scattering (RIXS), X-ray Magnetic Dichroism (XMD). Special attention will be given to the detail of the ARPES beamline to present the methods available along with its recent developments. Finally, current nanoARPES investigations on 2D materials will be presented.

Higher order van Hove singularities in quantum materials

Professor Joseph Betouras
Loughborough University, United Kingdom

Metals and Correlated Electron Systems 4, June 30, 2023, 15:00 - 17:00

Higher order van Hove singularities (HOVHS) and flat bands have attracted wide interest recently due to the major role they play in the formation of electronic phases in quantum materials. A classification scheme, the effect of disorder and a method to detect and analyze HOVHS have been developed. The theoretical progress has been accompanied by experimental results, e.g. in the case of $Sr_3Ru_2O_7$, the surface of Sr_2RuO_4 and kagome metals. Recent work will be reviewed and new results on the fate of spin density waves in the presence of HOVHS will be presented.

The role of symmetric off-diagonal exchange in Kitaev honeycomb antiferromagnets

Ioannis Rousochatzakis[1], Yang Yang[2], Natalia Perkins[2]
[1]Loughborough University, Loughborough, United Kingdom, [2]University of Minnesota, Minneapolis, USA

Magnetism 4, June 30, 2023, 15:00 - 17:00

Correlated materials with strong spin-orbit coupled 4d and 5d ions and bond-dependent anisotropic interactions have been at the forefront of experimental and theoretical search for quantum spin liquids (QSL) in recent years. In this talk, I will present our current understanding of the enigmatic instabilities of the Kitaev QSL that are driven by the symmetric off-diagonal exchange anisotropy Gamma, one of the most prominent perturbations in available materials.

Probing the heterogeneity of electronic structure at the nano- to atomic-scale at SuperSTEM

Sean Collins[1], Hage Fredik[2], Demie M Kepaptsoglou[3], Quentin M Ramasse[1]
[1]*University of Leeds, United Kingdom,* [2]*University of Oslo, Norway,* [3]*University of York, United Kingdom*

Facilities 2, June 30, 2023, 11:00 - 13:00

Across condensed matter systems, the effect of surface and local, nanoscale variations in atomic structure on the optical, electronic, and magnetic states is often limited to ensemble measurements. This talk will present recent progress at SuperSTEM, the EPSRC National Research Facility for Advanced Electron Microscopy, direct microscopic measurements and covering advances in nanometre to atomic resolution imaging and spectroscopy of phonons, excitons, and plasmons as well as valence electronic structure [1] and prospects for examining magnons [2]. These highlights will demonstrate the range of capabilities on offer for current and prospective users in hand with the staff expertise on site, alongside an overview of access routes (free at the point of use). Of particular note are the SuperSTEM capabilities for atomic resolution imaging and chemical analysis at 60 keV beam energies as well as <10 meV energy resolution now delivered in electron energy loss spectroscopy. Focused ion beam sample preparation is also available on site, and recent equipment upgrades including counting-type electron detectors for spectroscopy. Plans for future instrumentation for quantum materials research will also be discussed.

Two recent research areas will be featured: (A) Momentum- and atomically-resolved phonon spectroscopy, particularly highlighting localisation of phonon responses at point defects in two-dimensional materials [3,4] and (B) mapping vibrational [5] and excitonic excitations across interfaces and at extended defects in molecular solids, including small molecule organic semiconductors and metal–organic frameworks.

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Materials for energy and sustainability

Peter Littlewood
University of Chicago, United States

Plenary Session 2, June 30, 2023, 09:00 - 09:30

The last century's advances in information technologies have been propelled by the control of simple electronic materials (metals, insulators, and semiconductors) on increasingly small length scales, now having reached the nanoscale. Semiconductor devices are built via a top-down manufacturing process that is suitable for low volume manufacture. Nanostructured materials of many kinds will also be critical for the energy revolution, e.g. for applications including solar, electrical storage, lightweight components, water treatment, and catalysis. However these materials will need to be manufactured by the ton, or by the square kilometer, which will require us to obtain unprecedented control of functional materials synthesis and manufacture. Modelling, synthesis, and measurement will need to be combined synergistically to develop new materials at scale.

But this is a science problem and not just an engineering problem: there are some fundamental questions that we poorly understand, and many of these are in condensed matter physics. How do charged ions migrate in a correlated electronic material (battery cathodes)? Why is the electrocaloric effect generally so small and how would we make it bigger (solid state refrigeration)? Why are superionic conductors common for Na, Ag, and Hg compounds but rare for Li (battery electrolytes)? What controls the properties of phase change materials (information storage)? And perhaps some more exotic applications – can one build a non-reciprocal active material at the nanoscale made entirely of inorganic components (actuators, sensors)?

While condensed matter physics has played a major role in driving electronic technologies (for example solar cells), we have neglected entropic effects in 'hard' materials. I will argue that applying soft matter thinking to complex hard matter (and often strongly-correlated) systems can be fruitful.

The Making of the Modern World

Professor Carl Chinn

Evening Talk, June 29, 2023, 17:40 - 18:15

With high-rise towers, wide American-style roadways and underpasses, and futuristic shopping malls, Birmingham is a contemporary city from which the past seems to have been banished and where each generation knocks down the buildings put up by its predecessors. A city of change, adaptation and inventiveness, its modernity is heightened by a belief that Birmingham emerged suddenly almost from nothing as a creation of the Industrial Revolution. Yet whilst Birmingham is not a phenomenon of the modern world only and instead has deep roots, the catalyst for its rise to international prominence as one of Britain's most important manufacturing towns was the Industrial Revolution, whilst Birmingham itself was as much a catalyst for that dramatic social, economic, cultural, and physical transformation. Soon to be hailed as 'the city of a 1000 trades' and 'the workshop of the world', Birmingham's impact on the Making of the Modern World was profound, an achievement arising from the work of the many and not the privileges of the few.

Bringing Magnetic Order to Topological Insulators

Thorsten Hesjedal
University of Oxford, United Kingdom

M4QN Focus Session, June 29, 2023, 15:00 - 17:30

Topological quantum materials, specifically topological insulators (TIs), have shown great potential for spintronics, e.g., due to their significant spin-orbit coupling and their dissipationless, counter-propagating surface states. When combined with magnetic order, these materials can exhibit new quantum states, such as the quantum anomalous Hall effect, which was first observed experimentally in films of (Bi,Sb)2Te3 doped with Cr. However, magnetic doping can have adverse effects, resulting in the need for extremely low operational temperatures. As a result, alternative methods are being investigated, with proximity coupling to magnetically ordered systems being a viable option for raising the operational temperature for observing these quantum effects.

In my presentation, I will discuss the potential of TI heterostructures for tuning their magnetic and topological properties. Specifically, I will review proximity coupling and interfacial effects in these heterostructures. I will provide an overview of molecular beam epitaxy and magnetron sputtering for heterostructure growth, as well as the various techniques used for structural, electronic, and magnetic characterization. I will go beyond the commonly studied transition-metal-doped and undoped TI heterostructures and present examples of rare-earth-doped TIs, magnetic insulators, and antiferromagnets, which can give rise to intriguing phenomena such as skyrmions and exchange bias. Lastly, I will discuss some novel heterostructures, including intrinsic magnetic TIs and systems involving 2D materials, and cover the time-resolved measurement of spin dynamics in these systems.

Science and Technologies at the European Magnetic Field Laboratory

Professor Amalia Patanè
University of Nottingham, United Kingdom

Facilities 2, June 30, 2023, 11:00 - 13:00

This talk reviews recent advances at the European Magnetic Field Laboratory (EMFL) with focus on high magnetic fields as a powerful means of understanding and manipulating matter. Also, it describes opportunities available to researchers for collaborations with the EMFL.

The EMFL unites, coordinates and reinforces all existing European large-scale high magnetic field research infrastructures in a single body. It includes the Laboratoire National des Champs Magnétiques Intenses (LNCMI) with sites in Grenoble and Toulouse, the High Field Magnet Laboratory (HFML - Nijmegen) and the Hochfeld-Magnetlabor (HLD - Dresden) providing access to the highest continuous and pulsed magnetic fields in Europe. The HFML-Nijmegen and the LNCMI-Grenoble are committed to generate the highest continuous magnetic fields, currently up to 38 T. The HLD-Dresden and the LNCMI-Toulouse focus on non-destructive pulsed fields, currently up to 100 T, and semi-destructive fields up to 200 T. Besides the continuous improvement of the magnetic field strength, the EMFL focuses on the realization and accessibility of top-class experimental infrastructure. For example, magnetic fields can be used in conjunction with a free electron laser (FEL) at the HLD-Dresden (FEL-ELBE) and at the HFML-Nijmegen (FELIX). Also, novel experimental techniques, so far not often used in high fields, are under development at the EMFL, such as scanning-probe microscopy, high pressure and micro-calorimetry measurements.

Investigations of Skyrmion materials

Professor Geetha Balakrishnan
University of Warwick, United Kingdom

M4QN Focus Session, June 29, 2023, 15:00 - 17:30

Recently, there has been considerable interest in the physics of magnetic skyrmions due to their huge potential for use in spintronic devices, such as in racetrack memories and logic devices. Magnetic skyrmions are topological magnetic spin structures originally identified in the B20 class of materials. More recently, skyrmions have been found and investigated in other non-centrosymmetric classes of materials and in centrosymmetric intermetallics. To make headway in experiments to understand the basic physics of these skyrmion materials, high quality single crystals are essential. This has motivated us to embark upon a study of several classes of skyrmion materials and to explore a wide composition range of each of the family of compounds. The materials investigated range from centrosymmetric intermetallics such as Gd2PdSi3, GdRu2Si2, magnetic layered van der Waals materials such as Fe3GeTe2, to a large family of intercalated transition metal dichalcogenides (TMDCs).

In this talk, I will present an overview of the materials characteristics of several of the above materials including the challenges in the synthesis of these materials using a variety of techniques at Warwick. Investigations of the effects of substitution and the resulting structural order/disorder on the existence of the skyrmion phase in these crystals sheds light on the origin and the tuning of the skyrmion lattices. The study of their important structure–property correlations is vital to the understanding of these materials for potential future device applications.

Tuning dimensionality, magnetism and conduction in van-der-Waals Mott insulators TMPS3

Dr Matthew Coak
University of Birmingham, United Kingdom

Magnetism 2, June 30, 2023, 09:30 - 10:30

The van-der-Waals antiferromagnets TMPS3, where TM = Transition Metal, form an ideal playground for tuning both low-dimensional magnetic and electronic properties [1-4]. These are layered honeycomb antiferromagnetic Mott insulators, long studied as near-ideal 2D magnetic systems with a rich landscape of competing interactions and a variety of magnetic properties across the family.

I will give an overview of my work using high pressure as a continuous tuning parameter to control the dimensionality of these materials. Due to the weak physical inter-planar forces in such van-der-Waals materials, pressure gives us clean and selective control over the inter-planar spacing and hence interactions.

I will present magnetic, structural and electrical transport results and compare the behaviour of Fe-, V-, Mn- and NiPS3 as we tune them towards 3D structures – and Mott transitions from insulator to metal. I show multiple enigmatic features in electrical transport in this 'strange metal' high pressure regime. I will focus in particular upon my recent ultra-high-pressure neutron scattering results, which have unveiled an enigmatic form of short-range magnetic order in metallic FePS3. This phase is particularly important as it most likely forms a precursor to superconductivity, and the direct observation of magnetism here completely overturns the existing wisdom in the literature of a spin-crossover transition as the Fe local environment changes.

These neutron diffraction results made use of new cutting-edge experimental techniques [5] which have allowed measurements of magnetic structure through powder diffraction up to 20 GPa at the ILL - smashing the previous 10 GPa record. Piecing together our high-pressure neutron, transport and x-ray results has allowed us to map out the full phase diagram - a first in this crucial family of materials, and likely to become the archetypal example. We observe multiple transitions and new states, and an overall increase in dimensionality and associated changes in behaviour.

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Quantization of Macroscopic Phenomena

JC Seamus Davis
University of Oxford, United Kingdom

Vinen Memorial Session, June 29, 2023, 15:00 - 17:30

Quantum and classical mechanics are equally deterministic in terms of their state variables. But quantum state variables are complex-valued and thus (we believe) cannot represent 'real' observables in our world. Born hypothesized that the product of each such complex function with its conjugate represents the probability of 'real' occurrences. This, among many other extraordinary consequences, implies new topological constraints on 'reality'. For example, the fact that complex-phase must wind in integer multiples of 2π around any closed-loop trajectory results in quantization of microscopic angular momentum in units of $\hbar$. However, these topological constraints also pertain to macroscopic quantum states describable by complex fields, such as found in superfluids or superconductors. Feynman pointed out that complex-phase winding modulo 2π within a superfluid implies that the fluid circulation speed within a macroscopic torus should be quantized. It was Joe Vinen who first demonstrated that this extraordinary conjecture is borne out in nature (W.F. Vinen Nature 181 1524 (1958)). Here I will review Vinen's famous superfluid 4He circulation quantization research and then touch on his gracious and rewarding engagement during our search for circulation quantization in superfluid 3He (J.C. Davis et al PRL 66, 329 (1991)).

Magnetism on the stretched diamond lattice in lanthanide orthotantalates

Sian Dutton
University of Cambridge, United Kingdom

Topological Materials 2, June 30, 2023, 11:00 - 13:00

The magnetic lanthanide ions, Ln3+, in the fergusonite and scheelite crystal structures form a distorted or stretched diamond lattice which is known to host exotic magnetic ground states. In this talk I will present work exploring the synthesis and characterisation of fergusonite orthotantalates M−LnTaO4 (Ln = Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er). I will focus on TbTaO4 which is observed to order antiferromagnetically at 2.25 K and from neutron diffraction has a commensurate magnetic structure with k=0 and Tb3+ moments parallel to the b axis. The evolution of the magnetism with applied magnetic field will also be presented through combined neutron, magnetic susceptibility and heat capacity measurements.

Strain control of a bandwidth-driven spin reorientation in Ca3Ru2O7

Dr Cameron Dashwood
University of Cambridge, United Kingdom

Metals and Correlated Electron Systems 4, June 30, 2023, 15:00 - 17:00

The layered-ruthenate family of materials possess an intricate interplay of structural, electronic and magnetic degrees of freedom that yields a plethora of delicately balanced ground states. This is exemplified by Ca3Ru2O7, which hosts a coupled transition in which the lattice parameters jump, the Fermi surface partially gaps and the spins undergo a 90° in-plane reorientation. In this talk, I will show how the transition is driven by a lattice strain that tunes the electronic bandwidth. We applied uniaxial stress to single crystals of Ca3Ru2O7 using cells from Razorbill Instruments, combined with neutron scattering at ISIS and resonant x-ray scattering at the Diamond Light Source to simultaneously probe the structural and magnetic responses. These measurements demonstrated that the transition can be driven by externally induced strain, stimulating the development of a theoretical model by our collaborators in which an internal strain is generated self-consistently to lower the electronic energy. We understand the strain to act by modifying tilts and rotations of the RuO6 octahedra, which directly influences the nearest-neighbour hopping. Our results offer a blueprint for uncovering the driving force behind coupled phase transitions, as well as a route to controlling them.

Topology, superconductivity, excitons and ferroelectricity all in one place

David Cobden
University of Washington, United States

Plenary Session 1, June 29, 2023, 09:00 - 09:30

Graphite has been found to display an astonishing variety of electronic phenomena in the atomically thin limit. WTe2 is another layered semimetal that can also be prepared and studied in this limit, albeit with considerably more effort. WTe2 differs from graphite in important ways, having much lower symmetry and stronger spin-orbit coupling, and it turns out to be full of surprises of its own. In the monolayer it is not a semimetal but a two-dimensional topological insulator, possessing helical one-dimensional edge modes. The insulating state exhibits peculiar behavior indicative of excitonic correlations, and it undergoes a quantum phase transition to a superconducting state on electrostatic doping. In addition, thin WTe2 exhibits a previously unrecognized layer-sliding ferroelectricity that intermingles with its other properties. The surprises keep coming as we continue to explore this category of two-dimensional materials. For example, the closely related MoTe2 turns out to have its own unique properties.

Collective dynamics of ions and vortices in He II in experiments of Joe Vinen

Professor Ladislav Skrbek
Charles University, Czech Republic

Vinen Memorial Session, June 29, 2023, 15:00 - 17:30

Pools of positive and negative ions – tiny snowballs and bubbles – trapped by electric field underneath the surface of superfluid 4He (He II) serve as a playground of classical two-dimensional (2D) physics. We discuss various collective modes of response of these systems to ac drive and their interaction with surface waves – ripplons, leading to detection of 2D Coulomb crystals. Collective dynamics of line defects in He II – quantized vortices – represent the essential ingredient of quantum turbulence. Since its discovery in pioneering Vinen's experiments on thermal counterflow of He II, quantum turbulence became established as a fast developing research field and represents an intellectual challenge for many investigators. We discuss the long-standing puzzles on transition to quantum turbulence and its temporal decay set by these early experiments and recent progress in disentangling them.

Optimizing Materials in Superconducting Quantum Circuits

Martin Weides
University of Glasgow, United Kingdom

M4QN Focus Session, June 29, 2023, 15:00 - 17:30

Superconducting circuits, as principal components in quantum sensing and computing, rely significantly on advancements in materials science for improved performance and reliability. The progression in this field directly correlates with enhancements in sensing accuracies and prolongation of qubit coherence times, thus expediting the growth of quantum technologies.

Material selection and nano-fabrication processes for these superconducting devices have a direct influence on their functionality and dependability. Therefore, the development of suitable fabrication and film growth techniques is crucial for the integration of quality-engineered components.

Moreover, quantum technologies drawing on quantum spintronics, hybrid qubits, or spin and topological qubits, offer notable functionalities, but often necessitate some magnetic background field. This requirement poses a limitation on the performance of traditional superconducting materials like aluminium.

We will elucidate the performance evolution of qubits under the influence of an applied magnetic field, as well as discuss innovative methods for superconducting resonators and junctions.

W.F. (Joe) Vinen: a brief summary of Joe's career and his many achievements.

Dr Chris Muirhead
University of Birmingham, United Kingdom

Vinen Memorial Session, June 29, 2023, 15:00 - 17:30

In this talk, I will outline some of Joe's many contributions to physics. The talk will cover Joe's early years at Cambridge, but will concentrate mainly on his time here in Birmingham. I will refrain from talking about the details of the physics, important parts of which will be dealt with by the subsequent speakers in this session. My talk will be a personalised view of what it was like to work with Joe as a supervisee, as a colleague, and as a friend over some 40 years.

Spin-liquid-like states in perovskite-related phases

Dr Otto Mustonen
University of Birmingham, United Kingdom

M4QN Focus Session, June 29, 2023, 15:00 - 17:30

Magnetic materials can host exotic quantum ground states [1]. Quantum effects are enhanced when magnetic interactions are frustrated – they cannot all be satisfied at the same time – and when the magnetic cations have small moments such as spin = 1/2. Quantum spin liquids are one example of these exotic ground states. These materials do not magnetically order or freeze even at absolute zero, and instead the magnetism remains dynamic and correlated: like a liquid. In this talk, I will introduce Cu2+ double perovskites as potential hosts for spin liquids and show how their ground states can be tuned using nonmagnetic d10 and d0 cations [2-5].

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High-Magnetic-Field Studies of Hydride High-Temperature Superconductors

Dr Sven Friedemann
University of Bristol, United Kingdom

Superconductivity 3, June 30, 2023, 15:00 - 17:00

A new area of record superconductivity has been heralded by the discovery of superconductivity at 200 K in sulphur hydride SH3 in 2015 [1]. Since the initial discovery, further superconductors with transition temperatures up to 288 K have been reported in LaH10, YH9, and carbonaceous sulphur hydride [2–4]. Experimental studies of the superconductivity in hydride superconductors have only been reported by a hand full of groups owing to the enormous challenges to conduct experiments at pressures above 100 GPa in diamond anvil pressures cells. Here, I will present our recent experimental results on superconductivity in SH3, LaH4, and YH4. Our results provide the first independent confirmation of superconductivity in SH3 [5]. I will discuss results of detailed transport studies including in very high magnetic fields. In SH3, we find evidence for clean-limit superconductivity and discuss the effects of thermal fluctuations. For LaH4, we find forms of the critical field that suggest multiband superconductivity. I will discuss our unique experimental approach using thin-film techniques [6] in the preparation of samples for high-pressure studies and how these might allow further studies and potentially applications of hydride superconductivity.

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Calculating thermodynamics, magnons and spin currents in complex magnetic materials using atomistic spin dynamics

Joseph Barker
University of Leeds, United Kingdom

Magnetism 1, June 29, 2023, 09:30 - 10:30

Atomistic spin dynamics based on the classical Heisenberg model is the magnetic equivalent to molecular dynamics. It enables the calculation of equilibrium properties and non-equilibrium dynamics and finite temperatures. For a long time, temperature has been treated always in the classical limit, with a Rayleigh-Jeans distribution. However, the magnon Debye temperature is usually very high and of the same order as the Curie temperature. Therefore, the use of classical statistics is poorly justified. We have recently implemented a quantum heat bath for classical spin dynamics which dramatically changes the results of calculations and provides a new level of quantitative agreement with experiments [1]. I will introduce the general formalism. Then, using a multiscale approach [2] for the complex but widely used magnetic oxide, yttrium iron garnet, show how we can now calculate properties such as magnon heat capacity and magnon spin conductivity which are both extremely difficult to measure in experiments and cannot be calculated correctly with classical statistics.

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High-yield atomically precise fabrication using arsenic in silicon and germanium

Dr Taylor Stock
University College London, United Kingdom

Semiconductors, June 29, 2023, 09:30 - 10:30

Semiconductor device manufacturing is steadily approaching the ultimate limit of miniaturization – single-atom precision. Meeting the challenge of developing a scalable, atomically precise fabrication technique would afford tremendous scientific and technological opportunities. By providing completely new engineered quantum materials and devices, atomically precise fabrication can enable the exploration of new areas of condensed matter physics and the realization of solid-state quantum computers.

Scanning tunnelling microscopy hydrogen resist lithography is the only fabrication technique capable of positioning individual dopant atoms at nearly exact lattice sites in silicon and germanium. Traditionally, this technique has used the precursor phosphine to precisely position phosphorus atoms. Using phosphorus-in-silicon, single and few atom donor devices are now routinely being demonstrated, providing tantalizing glimpses into future quantum technologies. Recent studies, however, suggest that the phosphine-silicon surface chemistry limits the single-atom fabrication yield. Arsine as a precursor to arsenic patterning offers an alternative and advantageous approach to atomically precise fabrication [1,2]. By using arsenic-in-silicon it is possible to improve the single-atom yield sufficiently to provide pathways to single-atom precision fabrication scale-up. In this talk I discuss atomically precise fabrication using scanning tunnelling microscopy and share recent progress in high-yield single-atom arsenic patterning in silicon and germanium.

References:
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Surfactant-mediated epitaxial growth of large-area transition-metal dichalcogenides

Akhil Rajan
University of St Andrews, United Kingdom

Surfaces, Interfaces and Thin Films, June 30, 2023, 11:00 - 13:00

To improve our fundamental understanding of the exceptional optical, electronic and mechanical characteristics of 2D transition-metal dichalcogenides (TMDs), it is important to develop techniques for the growth of high-quality monolayer samples. Similarly, to gain full control and ultimate applications, it is necessary to combine TMDs in heterostructure geometries. These are normally fabricated using exfoliated layers from bulk crystals, which lacks deterministic thickness control and cannot be easily scaled. High-quality large-area synthesis is thus the first crucial step to exploit the functional properties of TMDs. In principle, growth via molecular-beam epitaxy (MBE) should be the premier route to achieve this. However, efforts to achieve this to date have been complicated low coverage, unfavourable morphologies, the onset of bilayer formation, and the presence of rotational disorder. Here, we demonstrate a novel method for 2D materials growth by MBE, via the use of foreign species to act as surfactants for the growth of large-area, uniform, epitaxial TMDs. While the influence of surface-active species in facilitating heteroepitaxial growth of conventional semiconductors is known, it has not been explored for 2D materials. Here, we study the role of surfactants on the growth rate, stabilisation and enhancement of layer-by-layer growth mode on various TMDs, identifying and optimising their influence in suppressing 3D island formation and increasing growth rate by means of additional nucleation sites and enhanced edge diffusion. Through this, we demonstrate improved crystalline quality and uniform monolayer surface coverage over extended areas, paving the way to the growth of epitaxial heterostructures of TMDs

From single to multi-gap topological materials

Dr Bartomeu Monserrat
University of Cambridge, United Kingdom

Topological Materials 2, June 30, 2023, 11:00 - 13:00

Topology has emerged as a powerful tool to understand and classify states of matter. Examples of topological materials include topological insulators, Chern insulators, and Weyl and Dirac semimetals. All these phases can be described by dividing the energy spectrum into two parts separated by a gap or by low-dimensional crossing points. In this context, we call this paradigm "single-gap topology". Over the past two years, the new paradigm of multi-gap topology, in which more than a single gap is required for the description of the system, has emerged as a new direction in the study of topological matter. Multi-gap topological phases host exotic phenomena such as bulk band nodes carrying non-Abelian charges. Despite growing interest, the experimental observation of multi-gap topology in real materials is still missing.

In this talk, I will describe single and multi-gap topology in materials. I will explore topological phenomena in both electron and phonon spectra, I will discuss the interplay of topology with external parameters such as temperature and strain, and I will present material candidates for multi-gap topological phases with associated experimental signatures.

XMaS: The UK Materials Science Facility at the ESRF

Dr Yvonne Grunder[1], Oier Bikondoa[2,3], Laurence Bouchenoire[1,3], Edgar Gutierrez- Fernandez[2,3], Olga Filimonova[1,3], Paul Thompson[1,3], Didier Wermeille[1,3], Malcolm Cooper[2], Chris Lucas[1], Tom Hase[2]
[1]University of Liverpool, United Kingdom, [2]University of Warwick, United Kingdom, [3]XMaS, France

Facilities 2, June 30, 2023, 11:00 - 13:00

XMaS [1] is a diffraction and spectroscopy beamline located at the European Synchrotron Radiation Facility (ESRF) in Grenoble since 1997. It is a designated EPSRC funded National Research Facility with the aim to provide the UK materials science community with access to a state of-the-art X-ray facility and to facilitate training for early career scientists in advanced scientific methodologies.

Although the beamline was originally designed for the exploration of magnetic materials using scattering techniques, it nowadays offers a wide range of x-ray techniques, ranging from diffraction over resonant and small angle scattering to spectroscopic methods (e.g. XAS, EXAFS). XMaS delivers X-ray characterisation methodologies across a range of temporal and spatial length scales and, by the development and use of novel sample environments, facilitates increasing use of operando studies enabling correlations between structure and functional properties to be determined.

The availability of different X-ray techniques allows a broad range of scientific areas to be tackled including soft matter, surface electrochemistry, hard condensed matter and magnetism, conservation of historical artefacts and medical materials.

XMaS has undergone an extensive upgrade through 2019 and 2020 to deliver a state-of-the-art facility that fully exploits the capabilities of the new upgraded ESRF machine. The new facility delivers a much brighter X-ray beam with an extended operational energy range up to ~40 keV thereby enabling new activities in materials research, particularly in terms of operando experiments.

The talk will present the beamline capabilities offered to users. Examples of recent experiments using (resonant) surface X-ray diffraction for electrochemical in-situ studies will also be presented. [2-4]

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High-Field Solid-State Nuclear Magnetic Resonance National Research Facility

Dr Dinu Iuga
University of Warwick, United Kingdom

Facilities 2, June 30, 2023, 11:00 - 13:00

The High-Field Solid-State NMR National Research Facility provides access to a 23 T (1 GHz) narrow bore (54 mm) and a 20 T wide bore (89 mm) spectrometers and probes capable of spinning samples at the Magic Angle at very high spinning frequencies (up to 150 kHz). The high magnetic field provides higher sensitivity and this opens new opportunities for NMR experiments on low gamma and low natural abundance isotopes (like 17O, 25Mg, 33S, 43Ca, 39K, 89Y etc). Also at high magnetic fields the resolution is enhanced with clear noticeable effect for 1H and quadrupolar nuclei. This benefits opens new opportunities for structural research on energy materials, bio-materials, pharmaceutical, biological materials and other materials. Under very fast MAS, the 1H spin echo life time becomes considerably longer opening up the possibility to investigate 1H-1H proximities or to detect other atoms in vicinity to 1H. The presentation showcases examples of enhanced resolution and sensitivity enabled by the 1 GHz NMR spectrometer and provides a basic description of some Solid-State NMR experiments performed at Magic Angle Spinning.

Solving the polar interface in superconducting nickelate thin films

Dr Berit Goodge[1,2], Benjamin Geisler[3], Kyuho Lee[4,5], Motoki Osada[4,5], Bai Yang Wang[4,5], Danfeng Li[4,5,6], Harold Y. Hwang[4,5], Rossitza Pentcheva[3], Lena F. Kourkoutis[1,2]

[1]Cornell University, United States, [2]Max Planck Institute for Chemical Physics of Solids, Germany, [3]University of Duisburg-Essen, Germany, [4]SLAC National Accelerator Laboratory, United States, [5]Stanford University, United States, [6]University of Hong Kong, Hong Kong

Magnetism 3, June 30, 2023, 11:00 - 13:00

The stabilization of superconducting infinite-layer nickelates provides a long-awaited experimental platform to explore a close analogue of the high-Tc cuprates. As the family of superconducting nickelate thin films grows, however, superconductivity remains unreported in bulk samples, raising questions about the origin of superconductivity in these samples. In particular, it was proposed that the strongly polar interface between the SrTiO3 substrate and RNiO2 films could give rise to a two-dimensional electron gas (2DEG) with even higher carrier density than the superconducting LaAlO3-SrTiO3 interface. Leveraging high-resolution electron energy loss spectroscopy (EELS) in the scanning transmission electron microscope (STEM), we reveal the atomic-scale lattice structure and charge distribution at the nickelate-substrate interface. Informed by systematically varied theoretical models, we provide a more complete understanding of the role played by this interface for superconductivity. This work offers key insights to both the origin of superconductivity in these materials and to the more general exploration of other strongly polar and interfacial systems.

Using negative ions to measure Joe Vinen’s energy barrier

Professor Peter McClintock
Lancaster University, United Kingdom

Vinen Memorial Session, June 29, 2023, 15:00 - 17:30

One of Joe’s early contentions was that there must exist an energy barrier impeding the ab initio creation of a quantized vortex line or ring in superfluid 4He. Experiments undertaken to measure this barrier based on the use of negative ions will be described. Comparison of the experimental barrier height with that calculated by Joe and his group yielded excellent agreement, thus providing a triumphant vindication of Joe’s physical picture of vortex creation through macroscopic quantum tunnelling.

Magnetic Charge Ordering in 3D Artificial Spin-ice

Dr Sam Ladak
Cardiff University, United Kingdom

Magnetism 4, June 30, 2023, 15:00 - 17:00

In this talk, I will outline experiments and modelling carried out upon a 3D artificial spin-ice system [1,2,3,4] which takes the geometry of a diamond-bond lattice, capturing the arrangement of spins in bulk pyrochlore systems. Monte-Carlo simulations of such structures, predict a rich phase diagram with a number of charge-ordered phases including a single and double charged monopole crystal [5]. By using magnetic force microscopy, I will show that the vertex states in experimental systems can be determined, and monopole transport upon the lattice surface can be directly visualised [2]. I will show that experimental demagnetised systems are found to host ferromagnetic stripes upon the surface, a configuration that forbids the formation of the expected double-charge monopole crystal ground state [5]. Instead, the system forms crystallites of single magnetic charge, superimposed upon an ice background. I will move onto discuss how the measured configuration can be understood in terms of an enhanced monopole chemical potential upon coordination-two vertices at the surface, and how this can be controlled with intricate 3D nanostructuring to realise the expected double-charge crystal ground state.

1. May, A. et al. Realisation of a frustrated 3D magnetic nanowire lattice. Communications Physics 2, 13 (2019)
2. May, A. et al. Magnetic charge propagation upon a 3D artificial spin-ice. Nature Communications 12, 3217 (2021)
3. Sahoo, S. et al. Observation of Coherent Spin Waves in a Three-Dimensional Artificial Spin Ice Structure. Nano Letters 21, 4629 (2021)
4. Van den Berg, A. et al. Combining two-photon lithography with laser ablation of sacrificial layers: A route to isolated 3D magnetic nanostructures, Nano Research 16, 1441 (2023)
5. Saccone, M. et al. “Exploring the phases of 3D artificial spin ice: From Coulomb phase to magnetic monopole crystal”, arXiv:2211.04551 (2023)

Deterministic Single Ion Implantation at the NIBC and the RAISIN Network.

Dr David Cox
University of Surrey, United Kingdom

Facilities 2, June 30, 2023, 11:00 - 13:00

The National Ion Beam Centre has been implanting ions for more than 40 years. Covering most of the periodic table and with accelerating energies up to MeV it has served both academic and industrial research from almost all corners of the world. The recent emergence of quantum technologies has led to many requests for increasingly lower ion doses down to the single ion level with high positional accuracy in the nm range. Historically, the IBC has dealt in implant doses in the range 1012 to 1017 ions/cm2 on the scale of semiconductor wafers and addressing this new challenge has led to the development of a whole new activity in the centre - The deterministic implantation of single ions. This talk will describe progress to date in this activity in the IBC, covering the new instruments themselves, the ion source development required for specific species, and detection of implants events at the single ion level.

In the last year Surrey has also formed an EPSRC funded international network RAISIN – Roadmap for Applications of Implanted Single Impurities Network. This network brings together researchers from around the world working in single impurities in the solid state. I will give details of this network, its activities and how it can fund access to the instruments at the NIBC and collaboration seed-funding to work with others in the network.

Enhanced surface magnetism in the ferromagnetic Sr4Ru3O10

Carolina De Almeida Marques
University of Zurich, Switzerland

Metals and Correlated Electron Systems 2, June 29, 2023, 11:00 - 13:00

Unconventional phases in strongly correlated electron materials such as superconductivity, density waves, magnetic order, and nematicity can be tuned by tiny external perturbations. This is illustrated by small changes to the lattice, charge, orbital and spin degrees of freedom resulting in the stabilization of new ground states, driven by electronic instabilities and changes to the underlying electronic structure.
The physical properties of strongly correlated electron materials are highly sensitive to tiny structural changes, as evidenced by experiments under hydrostatic pressure or uniaxial strain. This suggests that the relaxation occurring naturally at their surfaces provides opportunities to explore their properties in parameter regimes not accessible in the bulk. In the Ruddlesden-Popper series of the strontium ruthenates, clean single crystal surfaces exhibit increased octahedral distortions in the surface layer. In the bulk of the materials, the octahedral distortions result in increased electronic correlations and are one of the key ingredients to tune their properties from a superconductor without distortions in the single layer limit, to an isotropic ferromagnet with both rotations and tilts for the 3D compound. The electronic structure is tuned by these octahedral distortions, that can push van Hove singularities across the Fermi level and induce electronic instabilities. Using scanning tunneling microscopy and spectroscopy at ultra-low temperatures, we found that the surfaces of Sr2RuO4[1] and Sr3Ru2O7[2] both show a distinct ground state from the bulk materials, which is related to instabilities present in the bulk. In this talk, I will discuss the case of Sr4Ru3O10[3], a ferromagnetic material that undergoes a metamagnetic transition with in-plane magnetic field. By using a modest out-of-plane magnetic field, we control the position of a van Hove singularity. We use the energy of the Van Hove singularity to detect the surface magnetism and find a behaviour that is distinct from the bulk, providing an opportunity to understand its metamagnetism from microscopic information.

This work was done at the University of St Andrews in the group of Peter Wahl, in collaboration with W. Osmolska, I. Benedicic, L. C. Rhodes, M. Naritsuka (St Andrews), V. Granata, R. Arumugam , R. Fittipaldi and A. Vecchione (CNR SPIN).

References

[1] C. A. Marques et al., Magnetic-Field Tunable Intertwined Checkerboard Charge Order and Nematicity in the Surface Layer of Sr2RuO4, Adv. Mater. 33, 2100593 (2021).
[2] C. A. Marques et al., Atomic-scale imaging of emergent order at a magnetic-field-induced Lifshitz transition, Science Advances, 8, 39 (2022)
[3] C. A. Marques et al., Symmetry, spin and orbital character of a Van-Hove singularity in proximity to a Lifshitz transition in Sr4Ru3O10, arXiv:2303.05587 (2023)

Intrinsic magnetism in superconducting nickelate heterostructures

Dr Jennifer Fowlie
Stanford University, United States

Magnetism 3, June 30, 2023, 11:00 - 13:00

Nickel and copper are nominally very similar in chemistry so the search for superconductivity in nickelates is a story just as old as the quest to understand the high temperature superconductivity of the cuprates. A central feature of these efforts was to find a nickelate with a similar electronic structure to that of the cuprates and a significant part of this approach utilized thin films and heterostructures.

I will describe some of the most important advances made in the search for superconductivity in nickelates.

First, I will discuss the efforts made in the context of nickelate heterostructures and then I will introduce the recent discovery of superconductivity in infinite-layer nickelates [1] and the ever-growing family of nickelate superconductors.

Finally, I will come back to the comparison between nickelates and cuprates by examining what we have learned so far on the physics of the nickelates. In particular I will focus on results from x-ray scattering [2] and muon spin rotation [3] that suggest a coexistence of superconductivity and magnetism that may be as a result of the proposed multi-orbital nature of the nickelates.

[1] D. Li et al, Nature 572 (2019) 624
[2] H. Lu et al, Science 373 (2021) 213
[3] J. Fowlie et al, Nat. Phys. 18 (2022) 1043

EPSRC National Epitaxy Facility enabling semiconductor research in the UK

Dr Zofia Bishop[1], **Dr Edmund Clarke[1]**, Dr Elisa Sala[1], Dr Ian Farrer[1], Prof Rachel Oliver[2], Prof Huiyun Liu[3], Prof Maurice Skolnick[4], Prof Jon Heffernan[1]

[1]University Of Sheffield, Department of Electronic and Electrical Engineering, Sheffield, United Kingdom, [2]University of Cambridge, Department of Materials Science and Metallurgy, Cambridge, United Kingdom, [3]University College London, Department of Electronic and Electrical Engineering, London, United Kingdom, [4]University Of Sheffield, Department of Physics and Astronomy, Sheffield, United Kingdom

Facilities 2, June 30, 2023, 11:00 - 13:00

The EPSRC National Epitaxy Facility (NEF) is a Centre-of-Excellence for semiconductor epitaxy in the UK, established for more than 40 years. The Facility currently supports research grants in excess of £150m in over 25 UK universities and works with the UK semiconductor industry. We also offer advice in wafer structure design and undertake the growth development required to deliver custom-designed wafers to our users.

The Facility is a consortium of the Universities of Sheffield, Cambridge, and University College London and is home to 11 state-of-the-art epitaxial reactors, as well as a wide range of semiconductor characterization equipment. We specialise in the growth of III-V materials, group IV and hybrid group III-V/IV epitaxy. Our Pump Priming scheme allows researchers to conduct feasibility studies in support of grant applications. Through our new partnerships we offer epitaxy of emerging materials beyond the current III-V/IV provision. We are also expanding our capabilities into the field of heterogeneous integration with a new commercial Micro Transfer Print tool.

One example of our pioneering research is the growth of quantum dots (QDs) for quantum technology applications. Single InAs/GaAs QDs with linewidths of 2 μeV at 4 K have been realised and variation of growth conditions gives wavelength control from 900 to >1300 nm, with InAs/InP QDs providing emission from 1300 to 1600 nm. QDs incorporated into waveguides have demonstrated on-chip photon antibunching, resonance fluorescence and unidirectional spin transfer. Controlling the position of QDs using nanohole arrays enables scalable nanophotonic devices addressing multiple QDs.

SNOM lights up the nanoscale: non-destructive nanoscale optoelectronic characterisation via scattering-type Near-field optical microscopy

Dr Jessica Boland
University of Manchester, United Kingdom

1. Nonequilibrium Physics 2. Instruments and Applications, June 30, 2023, 15:00 - 17:00

Scattering-type scanning near-field optical microscopy (s-SNOM) has emerged as a promising new surface-sensitive technique for optoelectronic characterisation of low-dimensional materials. Here, an atomic force microscopy (AFM) tip is used to confine terahertz and midinfrared radiation to a volume defined by the radius of curvature of the tip, which is usually below 30 nm. When brought into contact with the tip, the evanescent near field interacts with the sample, encoding the local dielectric properties onto the THz wave. The tip then scatters the terahertz near-field back into the far-field, where it can be detected using conventional far-field techniques (e.g. electro-optic sampling). As the near-field signal is encoded with the local material dielectric properties, key electronic properties, including photoconductivity, mobility, and spin-dependent transport, can be examined on the nanoscale. But SNOM not only improves the spatial resolution by 3 orders of magnitude - it also offers surface sensitivity. By oscillating the tip and varying its amplitude, nanotomography can be performed to isolate surface and bulk contributions. A large tapping amplitude probes the bulk, whereas a small tapping amplitude probes the surface. In this talk, we demonstrate the use of s-SNOM in the midinfrared range to investigate the optoelectronic properties of topological insulators. We demonstrate the surface-sensitivity of the technique by performing nanotomography and demonstrate resonant responses at the surface of topological insulators. We also model the measured response using the finite dipole model to extract the localised dielectric function of the nanoparticles, highlighting the promise of this technique for nanoscale characterisation of a material's dielectric properties.

Structural signatures of metal-insulator transitions as seen by polarisation dependent x-ray absorption spectroscopy

Dr Silvia Ramos
University of Kent, United Kingdom

Metals and Correlated Electron Systems 2, June 29, 2023, 11:00 - 13:00

The absorption of linearly polarised X-rays is modulated by the relative orientation between the polarisation of the x-ray photons and the absorbing and scattering atoms. This property can be used to design synchrotron XAS experiments that measure local structure information as a function of the chemical species (as is the case with standard XAS measurements) and as a function of specific directions within the crystal structure. In this talk I will discuss this experimental technique and its application to the study of materials that display changes in conductivity but where a link to changes in the atomic structure has been challenging to confirm experimentally.

Electronic structure measurements of 2D materials, with a twist

Professor Neil Wilson
University of Warwick, United Kingdom

Helium and Complex Structured Materials, June 29, 2023, 11:00 - 13:00

A new parameter space to explore has been added to the beautiful world of 2D materials (2DMs), the twist angle between neighbouring layers. This is exemplified by ‘magic-angle’ twisted graphene, engineering strongly correlated behaviour through moire interactions, an effect also used to trap ordered arrays of excitons in transition metal dichalcogenide (TMDC) heterobilayers. Moire effects conventionally require a moire wavelength much longer than the atomic scale. But for larger lattice mismatch, Umklapp processes can result in unexpected electronic structure changes. Here, I will present our recent spatially-resolved angle-resolved photoemission spectroscopy studies of twisted 2DMs, including twisted graphenes and TMDCs. I will discuss initial-state and final-state effects, and the twist-angle dependence of inter-layer interactions.

Ion Implantation for Solid State Quantum Technologies

Prof Roger Webb
University of Surrey, United Kingdom

Facilities 2, June 30, 2023, 11:00 - 13:00

Solid-state quantum computation based on the intrinsic two-level dynamics of electron spin in semiconductors has attracted widespread attention because of the strong microelectronic integration. Ion beams, more specifically ion implantation, can be employed in the processing of solid state quantum devices in two ways.

The first is in Single Ion Implantation and a separate talk on this is given at this meeting by Dave Cox from the University of Surrey.

A second application is in the provision of isotopically pure substrates, more specifically in the process of Silicon Isotopic Enrichment. One important aspects of solid-state quantum devices dependent upon electronic spin and fabricated in silicon is that the donors must be isolated from environmental perturbations by being sited in a defect-free, cryogenically cooled, isotopically pure 28Si crystal which acts as a 'semiconductor vacuum'. Naturally abundant silicon has a 28Si content of 92.2%. 29Si atoms, with nuclear spin I = 1/2, occur at an abundance of ~4.7% and can disturb qubit states via nuclear spin interactions. 30Si atoms, which occur at 3.1% abundance, have no spin but their different mass can still cause localised magnetic field variations which hinder uniform nuclear magnetic resonance manipulation across all qubits. Reduction of the level of 29Si and 30Si or, conversely, enrichment of the level of 28Si, is therefore a key requirement for the realisation of silicon-based quantum computing. We have recently demonstrated the use of a conventional ion implantation to enrich a 28Si target to levels required for quantum devices. This has been achieved via two routes: i) direct implantation of an isotopically pure layer into the silicon substrate; and (ii) using a ion implantation into an Al film and using layer exchange to move the implanted, isotopically pure layer, to the surface of the silicon substrate. We will show the advantages and disadvantages of these techniques.

Fractional conductance in one-dimensional electrons

Dr Sanjeev Kumar
University College London, United Kingdom

M4QN Focus Session, June 29, 2023, 15:00 - 17:30

In a usual quantum wire, the conductance is quantised in units of 2e2/h. However, recent studies have shown that in asymmetrically confined quasi-one-dimensional quantum wires formed in GaAs/AlGaAs based heterostructures, the quantised conductance can appear at fractional values of e2/h without the presence of a quantising magnetic field. By relaxing the confinement potential of an electrostatically defined 1D quantum wire, the interacting 1D electrons form a zigzag pattern, resulting in fractional conductance states even in the absence of a magnetic field. In this presentation, we will demonstrate that when a 1D quantum wire is relaxed from symmetry to highly asymmetric confinement potential near the 1D-2D transition, conductance plateaus with both even and odd denominators (such as 1/6, 1/2, and 2/5) are formed. We will also discuss recent findings that suggest the Coulomb interactions between electrons can create correlated motion and cyclic current, leading to backscattering and the emergence of fractional conductance states [1-3].

References:
1. Kumar et al. Phys. Rev. Lett. 122, 086803, (2019); S. Kumar and M. Pepper, Appl. Phys. Lett. 119 110502 (2022).
2. Kumar et al., Appl. Phys. Lett. 115, 123104 (2019).
3. G. Shavit and Y. Oreg, Phys. Rev. Lett. 123 036803 (2019).

HarwellXPS – The UK National Facility for XPS; Analysis and Advances

Dr Mark Isaacs
University College London, United Kingdom

Facilities 2, June 30, 2023, 11:00 - 13:00

HarwellXPS has been the UK national facility for the past 5 years and in that time has earned a reputation for high quality analysis and training programs, raising the bar for XPS across the UK. Working with catalysis, battery materials, biomaterials, semiconductors and more, HarwellXPS is dedicated to providing high level access and support to researchers in need of surface analysis, regardless of experience. This talk will showcase the equipment and technologies available via HarwellXPS, demonstrate access policies and detail some of the recent scientific advances to come out of the facility.

New opportunities for Quantum materials research at the ISIS neutron and muon source

Pascal Manuel
ISIS Neutron and Muon Source, United Kingdom

Facilities 1, June 30, 2023, 09:30 - 10:30

ISIS Neutron and Muon Source is a world-leading centre for research at the STFC Rutherford Appleton Laboratory in Oxfordshire. It currently operates 34 neutron and muon instruments to give unique insights into the properties of materials over a wide range of lengthscales and timescales encompassing many topics from engineering to biology and soft matter as well as cultural heritage, energy materials, catalysis... This talk will focus on a few beamlines relevant for the condensed matter community, highlighting some recent works on complex experiments as well as the opportunities offered by our new beamline developments as part of the Endeavour programme [1] and the future facility: ISIS-II.

[1] https://www.isis.stfc.ac.uk/Pages/Endeavour.aspx

The Role of Quantum Computation in Condensed Matter Physics

Prof Andrew Green
University College London, United Kingdom

Metals and Correlated Electron Systems 2, June 29, 2023, 11:00 - 13:00

Quantum computers have tremendous promise for the study of many-body quantum systems. Applications in materials science and chemistry are amongst those with the most dramatic potential impacts. While the performance of quantum computers currently falls short of this promise, the pace of development is rapid. I will discuss the current state of the art and highlight the important role that condensed matter physics can play in driving this progress – providing a sequence of increasingly challenging target problems and refining our understanding of where improvements will be found.

Entropy of Quantum Materials

Dr Andreas W. Rost
University of St Andrews, United Kingdom

Metals and Correlated Electron Systems 1, June 29, 2023, 09:30 - 10:30

Many quantum materials studied extensively by the condensed matter community exhibit strongly correlated phases which can be tuned by e.g. magnetic field, uniaxial strain or pressure. By definition their thermodynamic behavior deviates from our standard expectations such as the Fermi liquid behaviour. Especially important is entropy, that directly links to the statistical physics of microscopic models. While measurements of changes of entropy with temperature are widely accessible and a standard experimental tool, changes of entropy as a function of tuning parameter such magnetic field (magnetocaloric effect) and uniaxial strain (elastocaloric measurements) are far less often utilized, although these can reveal unique insights into a material's properties.

In my talk I will briefly introduce these techniques and highlight their potential. As a recent application example I will discuss the phase diagrams of superconducting Sr2RuO4 as a function of uniaxial strain [1]. This material exhibits a superconducting dome controlled by a van Hove singularity (VHs) and in proximity to a magnetic phase. I will show how the elastocaloric effect can be used, for example, to study the strong entropy quench at the VHs upon entering the superconducting state, the evolution of the specific heat jump upon entering the superconducting phase, or the competition between superconductivity and magnetism.

Finally, I will explore how such measurements can be extended to wider range of quantum materials under uniaxial strain.

[1] Y.-S. Li et al. Nature 607, 276 (2022).

Contributed Talks

Magnetocondoctivity of CaC6 with a CDW-reconstructed Fermi surface

Petra Grozić[1]
[1]*University of Zagreb, Faculty of Science, Physics Department, Zagreb, Croatia*

Metals and Correlated Electron Systems 3, June 30, 2023, 09:30 - 10:30

The physics of intercalated graphite compounds (GIC), in spite of the fact that these materials have been synthesized quite long ago, is still in the focus of modern theoretical and experimental research. The interest of the scientific community is focused to GIC mostly due to the possibility to form the unusual superconducting (SC) and charge density wave (CDW) ground states.

We focus on one of these materials, CaC6, in which experiments clearly demonstrate existence of CDWs. The very existence of the CDW is quite unusual due to the fact that the graphene Fermi surface (FS), chemically doped by calcium intercalates, shoves no so-called "nesting property", i.e. no Peierls mechanism, which has been the paradigmatic mechanism leading to the CDW instability since 50s of the last century, and experimentally realized during 80s in the highly anisotropic materials with open Fermi surfaces.
We show that the CaC6 Fermi surface undergoes a different CDW formation mechanism, based on the topological reconstruction (of the FS) and critical strength of the electron-phonon interaction. Such topological reconstruction, that transforms the set of closed Fermi pockets to the open Fermi sheets, has profound effect of the transport and magnetotransport properties. We show the signature of the FS reconstruction by the CDW in the magnetotransport properties, taking into account magnetic breakdown, which shows characteristic quantum oscillations.

Non-Fermi Liquid Behaviour Induced by Gauge-Field Interactions: Insights from the Functional Renormalization Group

Mr Thomas Sheerin[1], Dr Chris Hooley[1]
[1]*School of Physics & Astronomy, University of St Andrews, St Andrews, United Kingdom*

Metals and Correlated Electron Systems 2, June 29, 2023, 11:00 - 13:00

Achieving a consistent and predictive theory of non-Fermi liquids in two spatial dimensions remains one of the key challenges of theoretical condensed matter physics. Due to strong correlations and the breakdown of the quasiparticle picture, little is known about the form of the low energy theories of such quantum-critical matter – exact identities, such as those implied by symmetries or anomalies, are thus invaluable for constraining the modelling. In this talk we will discuss the thermal field theory of a U(1) gauge field interacting with electrons at finite density, studied using the functional renormalization group (fRG). The Fermi liquid is known to be unstable to interactions with magnetic fields at sufficiently low temperatures [1], but all previous works have studied this phenomenon using perturbative techniques. The fRG is nonperturbative, and so can handle the strong interactions and non-analytic operators that naturally arise in such problems – the U(1) symmetry, on the other hand, provides constraints on low-energy correlators. We will detail how the associated Ward identities interplay with the choice of fRG regulators, and delineate a family of ansatze for the effective action that are explicitly gauge-invariant at all scales. We will then present RG flow equations for a number of these ansatze and discuss our attempts to find a stable, non-Fermi-liquid fixed point. We close by discussing the UV-IR mixing induced by gauge symmetry, as well as some potential future directions.

[1] M. Y. Reizer, Phys. Rev. B 40, 11571 (1989).

NanoFrazor Lithography for advanced 2D&3D nanodevices

Zhengming Wu[1]
[1]*Heidelberg Instruments Nano AG, Zurich, Switzerland*

1. Nonequilibrium Physics 2. Instruments and Applications, June 30, 2023, 15:00 - 17:00

NanoFrazor lithography systems were developed as a first true alternative or extension to standard mask-less nanolithography methods like electron beam lithography (EBL). Here a heatable ultra-sharp probe tip with an apex of a few nm is used for patterning and simultaneously inspecting complex nanostructures. The patterning depth of each individual pixel can be controlled with better than 1 nm precision using an integrated in-situ metrology method. Furthermore, the inherent imaging capability of the NanoFrazor technology allows for markerless overlay, which supports stitching layout sections together with < 20 nm error. Pattern transfer from such resist features below 10 nm resolution were demonstrated. The technology has proven its value as an enabler of new kinds of ultra-high resolution nanodevices as well as for improving the performance of existing device concepts. The application range for this new nanolithography technique spans from ultra-high resolution 2D and 3D patterning to chemical and physical modification of matter at the nanoscale. While patterning at below 10 nm resolution is achieved, an integrated laser write head for direct laser sublimation (DLS) of the thermal resist has been introduced for significantly faster patterning of micrometer to millimeter-scale features. The areas patterned by the tip and the laser are seamlessly stitched together and both processes work on the same resist material.
The presentation will include examples for (i) high-quality metal contacting of 2D materials, (ii) tuning photonic molecules, (iii) generating nanofluidic devices, (iv) generating spintronic circuits and (V) optical Fourier surfaces.

Exceptional points from two-photon driving

Dr. Charles Downing[1]
[1]*University Of Exeter, Exeter, United Kingdom*

1. Nonequilibrium Physics 2. Instruments and Applications, June 30, 2023, 15:00 - 17:00

The mathematical objects employed in physical theories do not always behave well. Within dissipative systems governed by matrices, singularities occur at the exceptional points in parameter space whereby some eigenvalues and eigenvectors coalesce simultaneously. However, the nature of exceptional points in truly quantum systems has been much less studied. Here we consider a quantum oscillator driven parametrically in an open quantum systems approach. This squeezed system exhibits an exceptional point in the dynamical equations describing its first and second moments, which acts as a borderland between two phases with distinctive physical consequences. In particular, we discuss how the populations, correlations, squeezed quadratures and optical spectra crucially depend on being above or below the exceptional point. We also remark upon the presence of a dissipative phase transition at a critical point, which is associated with the closing of the Liouvillian gap.

DC Transport and Magnetotransport Properties of the 2D Isotropic Metallic System with the Fermi Surface Reconstructed by the Charge Density Wave

Barbara Keran[1], Petra Grozić[1], Anatoly M. Kadigrobov[1,2], Zoran Rukelj[1], Danko Radić[1]
[1]Faculty of Science, Department of Physics, Zagreb, Croatia, [2]Ruhr-Universitaet Bochum, Theoretische Physik III, Bochum, Germany

Metals and Correlated Electron Systems 3, June 30, 2023, 09:30 - 10:30

We report the ground state stabilization and corresponding electrical transport and magnetotransport properties of the 2D metallic system with the isotropic Fermi surface reconstructed by the charge density wave. The onset of the charge density wave is spontaneous process, stabilized by the condensation energy gain due to the self-consistent mechanism of topological reconstruction of the Fermi surface and opening of the pseudo-gap around it. We address the signature of the uni-axial reconstruction in terms of the measurable quantities, such as the intra-band transport properties, including the one-particle density of states, the total and effective concentration of electrons and the Hall coefficient. Also, we analyze the magnetotransport properties of the system reconstructed by the bi-axial, checkerboard-like charge density wave, under conditions of magnetic breakdown. It manifests huge quantum oscillations in the diagonal components of magnetoconductivity, while the Hall conductivity changes sign varying the external magnetic field, with the finite region of vanishing Hall coefficient in between.

Activation of 2D polymerisation on inert surfaces with atomic clusters as extrinsic catalysts

Alessio Quadrelli[1], Leonardo Forcieri[1], Qingqing Wu[1], Songjun Hou[1], Barry Mangham[2], Neil Champness[3], David Buceta[4], Manuel Arturo López-Quintela[4], Colin Lambert[1], Samuel P. Jarvis[1]
[1]Physics Department, Lancaster University, Lancaster, United Kingdom, [2]School of Chemistry, University of Nottingham, Nottingham, United Kingdom, [3]School of Chemistry, University of Birmingham, Birmingham, United Kingdom, [4]Laboratory of Nanotechnology and Magnetism, University of Santiago de Compostela, Santiago de Compostela, Spain

Surfaces, Interfaces and Thin Films, June 30, 2023, 11:00 - 13:00

On-surface polymerisation has enabled the creation of a variety of covalently bonded 1D and 2D molecular structures on metal surfaces [1]. Despite rapid progress in this field, the fabrication of polymers on non-metal surfaces remains exceptionally challenging, particularly using thermal methods. Without a catalyst, precursor molecules sooner desorb from insulating surfaces before they can polymerise, greatly limiting our ability to prepare surface polymers on non-metal substrates where their properties could be better exploited. Although other strategies have been employed to produce high-quality networks, such as using light to initiate polymerisation [2], the more general method of thermal activation remains an attractive option for surface polymerisation of a greater variety of molecules.

Here we report the on-surface polymerisation of tetra (4-bromophenyl) porphyrin (Br_4TPP) using atomic quantum clusters (AQCs), just five atoms in size and stabilised by an oxygen layer, as extrinsic catalysts [3]. Using temperature-programmed X-ray photoelectron spectroscopy (TP-XPS) and high-resolution atomic force microscopy (AFM), our findings show that AQCs substantially reduce the activation temperature for polymerisation, resulting in a covalent network on inert and metal surfaces that survives ambient conditions. Density functional theory (DFT), climbing image nudged elastic band (CI-NEB), and dimer analysis highlights a strong dependence between the catalytic activity of AQCs and their stabilising oxygen layer, highlighting the potential to further tune the catalytic activity of these sub-nanometric catalysts.

[1] Grill et al. Nat Chem 12, 115-130 (2020).
[2] Lackinger, Dalt. Trans. 50, 10020 (2021).
[3] Forcieri et al. (Under review) (2023)

Topological Physics in Coaxial Cable Networks

Professor D.M. Whittaker[1], Ms M.M. McCarthy[1]
[1]*University Of Sheffield, Sheffield, United Kingdom*

Topological Materials 2, June 30, 2023, 11:00 - 13:00

The most interesting Hamiltonians of topological physics are those with the symmetries of random matrix theory, such as chiral and particle-hole symmetry. However, there are a limited number of physical realisations which exactly display these symmetries, particularly in topological photonics, where it is hard to suppress all symmetry breaking couplings. To explore fully the topological properties, it is also necessary to ensure that disorder can be introduced without breaking the relevant symmetries.

We show that networks of coaxial cables are an excellent system for experiments in topological physics. Radio frequency transmission in such a network can be described using a Hamiltonian formulation, with the state vector consisting of the voltages at each of the cable junctions. The matrix elements of the Hamiltonian are determined by the impedances of the corresponding cables. This provides a `lego' for topological physics: given a Hamiltonian, we can construct the corresponding network, and measure properties such as transmission and the local density of states at any point. Disorder can readily be introduced by swapping in cables with different impedances.

We shall give a live demonstration of the cable system, showing the physics of the SSH model in a structure consisting of sections of cable with two different impedances. We shall also show results demonstrating topological protection in an ensemble of random cables, and extend this to networks by looking at graphene and Lieb lattice structures.

Ambient characterisation of atomic defects in transition metal dichalcogenides with single atom resolution

Edward Dunn[1], Prof Robert Young[1], Dr Samuel Jarvis[1]
[1]*Lancaster University Physics Department, Lancaster, United Kingdom*

Surfaces, Interfaces and Thin Films, June 30, 2023, 11:00 - 13:00

Defects have been shown to be critical in understanding the properties of monolayer transition metal dichalcogenides (TMDs) [1]. Monolayer TMDs are thought to be promising candidates for a number of proposed nascent technologies, including quantum security devices [2], hydrogen evolution reaction catalysts [3] and transistors [4]. It is therefore essential to characterise the intrinsic defects of mechanically exfoliated TMDs and to be able to tune material properties by the introduction of new defects.
Here we show that conductive atomic force microscopy (cAFM) carried out in ambient conditions can achieve `true' atomic resolution on 2D-TMD materials. We show that it is possible to identify single-atom defects and subtle changes in the density of states of the surrounding nearest neighbour atoms. Furthermore, we show that specific defect types can be identified which we attribute to metal and chalcogen substitutions, and compare their appearance and frequency across multiple 2D-TMD materials (see Figure 1). In particular, we will show the relevance of atomic defects to optical properties by introducing new defects via exposure to nitrogen plasma. Changes in the defects observed in cAFM images are then compared with the changes in the optical signal to establish the nanoscale origins of these effects.

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Probing the superconducting transition in 2D materials with graphene-based SQUIDs

Emily Gamblen[1,2], Prof Roman Gorbachev[2], Dr Xiao Li[2], Mr Max Taylor[1,2], Dr Michael Thompson[1], Dr Jonathan Prance[1]

[1]Physics Department, Lancaster University, Lancaster, United Kingdom, [2]Department of Physics and Astronomy, University of Manchester, Manchester, United Kingdom

Superconductivity 2, June 29, 2023, 11:00 - 13:00

Superconducting 2D materials are providing insight into the fundamental physics of superconductivity, with potential applications in both quantum computing and conventional electronics. There are often significant differences in the electronic and magnetic characteristics of few- and monolayer materials when compared to bulk material. Two-dimensional superconductors are often far smaller in at least one dimension than the magnetic penetration depth of the bulk material, and therefore may not exhibit the Meissner effect which is characteristic of bulk superconductors.

We present measurements of the magnetic response of few-layer superconductor NbSe2 as it undergoes the superconducting transition. We will briefly discuss the design and properties of bespoke graphene-based superconducting quantum interference devices (SQUIDs) which are essential to this work.

Fractional Shapiro steps in graphene SQUIDs

Mr Max Taylor[1,2], Professor Moshe Ben Shalom[2,3], Ms Emily Gamblen[1,2], Dr Jonathan Prance[1], Dr Michael Thompson[1]

[1]Physics Department, Lancaster University, Lancaster, United Kingdom, [2]National Graphene Institute and Department of Physics and Astronomy, University of Manchester, Manchester, United Kingdom, [3]School of Physics and Astronomy, Tel Aviv University, Tel Aviv, Israel

Superconductivity 2, June 29, 2023, 11:00 - 13:00

When the characteristic frequency of a Josephson junction (JJ) matches an applied ac field, Shapiro steps appear in the current-voltage characteristic at voltages corresponding to integer multiples of the magnetic flux quantum proportional to the frequency of the applied field.

This phenomenon has been observed in many JJ systems, allowing for variations in the behaviour of Shapiro steps to be discovered. This includes the appearance of half-integer steps through a variety of proposed mechanisms. One of these is related to the current-phase relation (CPR) of the JJ, as if it deviates from the ideal sinusoidal form then higher harmonic terms could also lead to the formation of a step in the I-V[1]. Alternatively, in a dc superconducting quantum interference device (SQUID) formed from two JJs in parallel, half steps appear from changing the applied magnetic field[2].

We explore these mechanisms in simulation and experiment, using a numerical resistively and capacitively shunted junction (RCSJ) model for the former and a graphene SQUID for the latter. Graphene JJs and SQUIDs have been shown to have sinusoidal CPRs at charge neutrality but when electrostatically gated the CPR becomes significantly skewed[3,4]. Therefore, this system should be able to show the effect on Shapiro steps from both an applied magnetic field and the change in the CPR.

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Possible role of higher order singularities in Sr2RuO4 – a theoretical perspective

Anirudh Chandrasekaran[1], Prof Joseph Betouras
[1]*Loughborough University, Loughborough, United Kingdom*

Metals and Correlated Electron Systems 4, June 30, 2023, 15:00 - 17:00

In this talk, I will discuss a concrete paradigm for exploring, diagnosing, and engineering higher order Van Hove singularities (HOVHS) in the bandstructure of quantum materials, that was recently developed by us. The method has wide applicability, with target models ranging from simple few-band tight-binding models to detailed models based on ab-initio calculations. I shall illustrate the technique by applying it to the case of the surface states of Sr2RuO4 where, as I will demonstrate, the system is very close to attaining a pair of symmetry related, power-law diverging HOVHS at the M point. This is reminiscent of the HOVHS that occurs in Sr3Ru2O7, with its signatures manifesting in the thermodynamic properties of that material. This further leads to the question on the role of HOVHS in the properties of Sr2RuO4, which will be briefly addressed.

The Double-Q Ground State with Topological Charge Stripes in the Centrosymmetric Skyrmion Candidate GdRu2Si2

George Wood[1], Dmitry Khalyavin[2], Daniel Mayoh[1], Juba Bouaziz[3], Amelia Hall[1], Sam Holt[4,5], Fabio Orlandi[2], Pascal Manuel[2], Stefan Blu¨gel[3], Julie Staunton[1], Oleg Petrenko[1], Martin Lees[1], Geetha Balakrishan[1]
[1]Department of Physics, University Of Warwick, Coventry, United Kingdom, [2]ISIS Facility, STFC Rutherford Appleton Laboratory, Harwell Science and Innovation Campus, United Kingdom, [3]Peter Gru¨nberg Institut and Institute for Advanced Simulation, Forschungszentrum Ju¨lich & JARA, Germany, [4]University of Southampton, Southampton, United Kingdom, [5]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, Germany

Magnetism 4, June 30, 2023, 15:00 - 17:00

The stabilisation of skyrmions and topologically non-trivial spin textures in centrosymmetric intermetallics is highly topical. This is not only to understand the intricate interactions that can lead to these complex ordered states, but also because in this class of materials, there is a serious prospect of developing a useful spintronic device which uses the range of emergent phenomena in these systems. $GdRu_2Si_2$ is one such centrosymmetric material, which hosts a variety of exotic magnetic phases and may be considered a prototypical example, due to its simple structure [1].

Here, we present neutron diffraction on single crystal and polycrystalline $^{160}GdRu_2Si_2$ in which we have discovered a new double-Q incommensurate magnetic ground state [2]. In addition to observing the q_1 and q_2 propagation vectors, we have found magnetic satellites of the form q_1+2q_2. The appearance of these satellites are explained within the framework of a constant moment solution which is quantitatively refined. The structure, which contains vortex-like motifs, is shown to have a novel one-dimensional topological charge density. More generally, this work establishes that $GdRu_2Si_2$ has a wealth of topologically non-trivial spin textures and is therefore an ideal setting in which phase transitions between distinct topological structures can be experimentally probed.

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Structure and Phase Transformations of Metastable Hexagonal Uranium Thin Films

Dr Rebecca Nicholls[1], Dr Chris Bell[1], Dr Ross Springell[1], Dr Johann Bouchet[2], Professor Gerard Lander[1]
[1]*University Of Bristol, Bristol, United Kingdom,* [2]*CEA, DES, IRESNE, DEC, SESC, LM2C, F-13108 Saint Paul lez Durance, France*

Surfaces, Interfaces and Thin Films, June 30, 2023, 11:00 - 13:00

The ground state structure of bulk uranium metal is a low symmetry orthorhombic structure (α-U) which hosts several charge-density wave and superconducting states below 43 K [1]. At elevated temperatures, uranium can also adopt tetragonal (β-U, 935-1045 K) and body-centred cubic (γ-U, 1045-1405 K) structures. A fourth allotrope lies outside of the bulk phase diagram, with thin layers of uranium deposited onto either W(110) or Gd(00.1) forming a 'hexagonal close-packed' structure that is predicted to be dynamically unstable [2-3]. Little is known of the structural and electronic properties of this elusive hexagonal phase, as its crystallisation is unpredictable and its lattice parameters vary by almost 10% across published literature.

Here, we show that the room temperature sputter deposition of uranium onto Cu{111} or Ir{111} consistently promotes the growth of metastable (00.1)-oriented 'hexagonal close-packed-like' layers across a range of thicknesses (17.5-280 nm). X-ray diffraction and reflectivity measurements revealed that the malleable, strongly anisotropic (c/a = 1.80 - 1.92) layers gradually transition back into α-U in the days following growth. The complex, thickness dependent relationships relating the initial hexagonal structure and the final orientation(s) of α-U do not agree with the previously predicted transition mechanism [4] and so new transition pathways have been explored.

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Signatures of Supersymmetry in the ν=5/2 Fractional Quantum Hall Effect

Songyang Pu[1], Ajit Balram[2], Mikael Fremling[3], Andrey Gromov[4], Zlatko Papic[1]
[1]University of Leeds, Leeds, United Kingdom, [2]Institute of Mathematical Sciences, , India, [3]Utrecht University, Netherlands, [4]University of Maryland, College Park, U.S.A

Topological Materials 2, June 30, 2023, 11:00 - 13:00

The Moore-Read state, one of the leading candidates for describing the fractional quantum Hall effect at filling factor ν=5/2, is a paradigmatic p-wave superconductor with non-Abelian topological order. Among its many exotic properties, the state hosts two collective modes: a bosonic density wave and a neutral fermion mode that arises from an unpaired electron in the condensate. It has recently been proposed that the descriptions of the two modes can be unified by postulating supersymmetry (SUSY) that relates them in the long-wavelength limit. Here we extend the SUSY description to construct wave functions of the two modes on closed surfaces, such as the sphere and torus, and we test the resulting states in large-scale numerical simulations. We demonstrate the equivalence in the long-wavelength limit between SUSY wave functions and previous descriptions of collective modes based on the Girvin-MacDonald-Platzman ansatz, Jack polynomials, and bipartite composite fermions. Leveraging the first-quantized form of the SUSY wave functions, we study their energies using the Monte Carlo method and show that realistic ν=5/2 systems are close to the putative SUSY point, where the two collective modes become degenerate in energy.

Plasmons in a bilayer cuprate

Mr Jacopo Radaelli[1]
[1]*University Of Bristol, Bristol, United Kingdom*

Metals and Correlated Electron Systems 1, June 29, 2023, 09:30 - 10:30

The long-range nature of the screened coulomb interaction allows for dispersive charge excitations, known as plasmons, to appear in metals. Simple metals like copper have plasmons with gaps of several eV in the long wavelength limit. In contrast, systems made up of 2-D conducting layers separated by dielectric blocks show plasmons that disperse to zero energy when the wavevector component perpendicular to the layers is nonzero.

Cuprate superconductors approximately fit this mould by virtue of their largely decoupled electron/hole doped layers . However, acoustic plasmons have only recently been observed in single layer (one CuO_2 plane per unit cell) cuprates using resonant inelastic x-ray scattering (RIXS) at energies low enough to potentially play a role in the cuprates' unusual properties. Here we report the first RIXS measurement of dispersing plasmons in a bilayer cuprate (YBa2Cu3O6+x, Tc=89.9).

We carried out RIXS measurements at the O-K edge (1s -> 2p transition) with incident energy tuned to the oxygen holes responsible for conduction in hole-doped cuprates. We detect a weak dispersing plasmon with a relatively large ~300meV gap which is L dependent. Comparing our results with a correlated plasmon model, we conclude that a sizeable electronic coupling (t) between neighbouring CuO_2 planes in the bilayer must be included to understand this plasmon. This is in contrast to the single-layer case where neighbouring CuO_2 plane have only a small additional coupling (tz). [2]

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Correlated superfluidity produced by Floquet driving

Dr Charles Creffield[1], Mr Jesús Mateos, Dr Gregor Pieplow, Dr Fernando Sols
[1]*Complutense University Of Madrid, Madrid, Spain*

Atomic, Molecular and Optical Physics, June 30, 2023, 09:30 - 10:30

We study a one-dimensional Bose-Hubbard model in a lattice, and consider driving the kinetic energy periodically in time to realize a novel form of Floquet engineering termed "kinetic driving". At high frequencies, the driven system can be described by an effective static Hamiltonian in which the conventional single-particle hoppings vanish [1]. As a result, the dynamics is wholly governed by multi-particle correlations. For low driving amplitudes the system is a Mott insulator, but as the amplitude is increased it makes a quantum phase transition to an exotic superfluid state dominated by the preferential occupation of the lattice momenta $\pm\pi/2$. We discuss how this non-equilibrium superfluid phase differs qualitatively from conventional superfluidity [2,3], and contrast the phase transition with that seen in the standard Bose-Hubbard model, by analysing the spectral statistics of the system's quasienergy spacings.

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Magnetic penetration depth measurements of the superconducting energy gap structure of UTe2

Morgan Grant[1], Callum Stevens[2], Andrew Huxley[2], Antony Carrington[1]
[1]*University Of Bristol, Bristol, United Kingdom,* [2]*University of Edinburgh, Edinburgh, United Kingdom*

Superconductivity 3, June 30, 2023, 15:00 - 17:00

Thought to be in close proximity to a ferromagnetic instability, superconducting UTe_2 exhibits a spin-triplet pairing state, as evidenced by an upper critical field well-above the Pauli limit and NMR Knight shift measurements. Additionally, numerous re-entrant superconducting phases appear in the presence of an applied magnetic field and under pressure, the nature of which are yet to be understood. Necessary to understand the mechanism and pairing state of superconductivity in any material is knowledge of the superconducting energy gap structure, which aids in developing microscopic theories of the pairing interaction. Here, we report measurements of the anisotropy of the temperature dependence of the magnetic penetration depth in the Meissner state, a well-established probe of the gap structure. A ubiquitous T^2 dependence is observed, in contrast to the anisotropy expected for the suggested point-nodal state in the clean limit. The implications of this for other gap structures as well as the role of disorder are discussed.

Absence of thermalisation in a quantum dot

Mr George McArdle[1], Rose Davies[2], Igor Lerner[1], Igor Yurkevich[2]
[1]*University of Birmingham, United Kingdom,* [2]*Aston University, United Kingdom*

1. Nonequilibrium Physics 2. Instruments and Applications, June 30, 2023, 15:00 - 17:00

Electrons on a quantum dot fail to thermalise if the decay rate of quasiparticles on the dot is much less than the tunnelling rate to the leads. Such a regime is of particular importance at sufficiently low energies such that localisation in Fock space occurs [1] – a regime analogous to that of many-body localisation. We have investigated the impact made by the absence of thermalisation on the current-voltage (I-V) characteristics in the standard Coulomb blockade regime [2, 3].

For strong asymmetry in the coupling to the leads, we have demonstrated in [4] that the absence of thermalisation has no impact on the staircase in the I-V characteristics providing that the Fermi energy of the electrons on the dot is large in comparison to the charging energy (Fig. 1(a)). However, for a small Fermi energy, we have shown that the involvement of the lowest energy levels of the dot dramatically alters the transport properties, practically causing the disappearance of the staircase.

In the case of approximately equal coupling to both leads, we determined in [5] that the absence of thermalisation causes the distribution function of electrons on the dot to change from a Fermi function to a double-step form, similar to that seen in one-dimensional wires [6]. This manifests itself experimentally as an additional jump in the differential conductance (Fig. 1(b)).

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Two component charge fluctuations in La2-xSrxCuO4

Charles Tam[1,2], Mengze Zhu[1], Jaewon Choi[2], Stefano Agrestini[2], Kejin Zhou[2], Stephen Hayden[1]
[1]*University of Bristol, Bristol, United Kingdom,* [2]*Diamond Light Source, Didcot, United Kingdom*

Superconductivity 1, June 29, 2023, 09:30 - 10:30

With advances in soft x-ray optics and brilliance of light sources, the presence of charge density waves (CDW), and especially the presence of incommensurate charge fluctuations (CF) are now known to be a common feature of the cuprate superconductors. However, finding a coherent phenomenology independent from material dependence has proven tricky. In this contribution, I present measurements of CDW in the prototypical cuprate La2-xSrxCuO4 using Cu-L3 and O-K resonant inelastic x-ray scattering. We conduct a thorough doping dependence study, from x=0.11 to x=0.22, measuring the CDW both in Cu orbitals and in O orbitals (via Cu-O hybridisation).

We find the CDW and CF can be interpreted with two components. The first is a quasi-elastic component that is strongly associated with spin density wave and the dip in Tc at x=1/8, and is more characteristic of long range order. This component disappears near optimal doping x=0.16. The second component is more than likely inelastic, with energy scales with an upper bound limited by instrumental resolution (27 meV) and a reduced correlation length compared to the quasi-elastic component. The inelastic component spans the phase diagram that disappears between $0.19<x<0.22$. Both components are detected simultaneously in both Cu and O orbitals. This work provides key information on the CDW phenomenology in the cuprates which may help explain their unconventional nature.

On the Electron Pairing Mechanism of Copper-Oxide High Temperature Superconductivity

Wangping Ren[1], Dr. Shane O'Mahony[2], Dr. Weijiong Chen[1], Dr. Yi Xue Chong[3], Dr. Xiaolong Liu[3], Prof. H. Eisaki[4], Prof. S. Uchida[5], Dr. M.H. Hamidian[3], Prof. J.C.Seamus Davis[1,2,3,6]

[1]University of Oxford, Oxford, United Kingdom, [2]University College Cork, Cork, Ireland, [3]Cornell University, Ithaca, United States, [4]National Institute of Advanced Industrial Science and Technology, Tsukuba, Ibaraki, Japan, [5]University of Tokyo, Tokyo, Japan, [6]Max-Planck Institute for Chemical Physics of Solids, Germany

Superconductivity 1, June 29, 2023, 09:30 - 10:30

The elementary CuO_2 plane sustaining cuprate high-temperature superconductivity occurs typically at the base of a periodic array of edge-sharing CuO_5 pyramids. Virtual transitions of electrons between adjacent planar Cu and O atoms, occurring at a rate $t/\hbar$ and across the charge-transfer energy gap ε, generate 'superexchange' spin-spin interactions of energy J in an antiferromagnetic correlated-insulator state. However, hole doping this CuO_2 plane converts this into a very high temperature superconducting state whose electron-pairing is exceptional. A leading proposal for the mechanism of this intense electron-pairing is that, while hole doping destroys magnetic order it preserves pair-forming superexchange interactions governed by the charge-transfer energy scale ε. To explore this hypothesis directly at the atomic scale, we combine single-electron and electron-pair (Josephson) scanning tunnelling microscopy to visualise the interplay of ε and the electron-pair density n P in Bi2Sr2CaCu2O8+x. The responses of both ε and n P to alterations in the distance δ between planar Cu and apical O atoms are then determined. These data reveal the empirical crux of strongly correlated superconductivity in CuO_2, the response of the electron-pair condensate to varying the charge transfer energy. Concurrence of predictions from strong-correlation theory for hole-doped charge-transfer insulators with these observations indicates that charge-transfer superexchange is the electron-pairing mechanism of superconductive $Bi_2Sr_2CaCu_2O8+x$.

Designing organic/2D heterostructures for photovoltaic applications

Dr Juliana Morbec[1], Mr Edward Black[1]
[1]*Keele University, United Kingdom*

Surfaces, Interfaces and Thin Films, June 30, 2023, 11:00 - 13:00

Combining two-dimensional (2D) materials with organic materials can be very attractive for applications that require flexibility and where size and weight are important parameters to be considered, such as in wearable, portable and mobile applications. Organic materials usually exhibit excellent optical absorption efficiency and photo- and temperature-induced conformational changes, while 2D materials often show relatively high carrier mobility, superior mechanical flexibility, and tunable electronic and optical properties. Combining both systems can stabilize the organic materials and lead to heterostructures with both high carrier mobility and high optical absorption efficiency, which is promising for solar energy conversion.
In this work we investigate, by means of density-functional-theory calculations, heterostructures composed of organic molecules (for example, pentacene and azulene) and transition metal dichalcogenides (TMD) for application in photovoltaic devices. We examine the interaction between the molecules and monolayer TMDs as well as the band alignment of the heterostructures, considering effects of the molecular coverage, rotation and dielectric screening.

Strong Coupling and Entanglement in Extreme Nanophotonic Cavities

Angus Crookes[1], Dr Ben Yuen[1], Dr Stephen Hanham[1], Dr Angela Demetriadou[1]
[1]*University of Birmingham, Birmingham, United Kingdom*

Atomic, Molecular and Optical Physics, June 30, 2023, 09:30 - 10:30

Quantum networks exploit both local and global entanglement across separate but connected quantum nodes to provide unbreakable encryption and scalable computation[1]. However, most high-fidelity local nodes are only weakly coupled to the electromagnetic field, limiting the entanglement rate[2]. Strong coupling between light and matter in photonic devices has the potential to increase entanglement rates by several orders of magnitude. Despite this, most devices operate at telecommunication wavelengths and lack a scalable architecture for use in an expansive network, making them unsuitable for realizing entanglement at optical frequencies[3].

In this work, we design photonic crystal waveguides that overcome these challenges, commanding unprecedented optical confinement and strong field enhancements while operating at 780 nm for entanglement with cold atoms (e.g. Rb). Unlike most other cavities, our designs are both high-finesse ($Q = 10^7$) and achieve subwavelength mode volumes, easily reaching deep into the strong coupling regime. Through the entropy dynamics of two emitters, we demonstrate local multi-partite entanglement generation, that is robust to displacement of the trapped atoms. The scalable architecture of our photonic crystal designs is also ideal for constructing networks with large numbers of qubits, where both local and remote entanglement can be realized.

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Termination-dependent surface states and bulk band structure of LaTe2

Alex Louat[1], Matthew D. Watson[1], Timur K. Kim[1], Cephise Cacho[1]
[1]*Diamond Light Source, United Kingdom*

Metals and Correlated Electron Systems 3, June 30, 2023, 09:30 - 10:30

The van der Waals (vdW) LaTe3 compound has been extensively studied for its nesting-driven charge density wave (CDW). The low energy physics comes mainly from the Te-sheets that happen to be the unique termination possible when cleaved. Whereas its cousin material LaTe2 is not a vdW material allowing two different surface terminations visible on Fig. 1a. The predicted charge imbalance at the surface is expected to manifest itself in potential surface states. The previous Angle-resolved photoemission (ARPES) studies [1,2] reported on LaTe2 lacked spatial resolution to be able to resolve the different termination preventing to identify the origin of the broad bands measured.

In this study, we investigate the termination-dependent bulk band structure and surface state using micro-ARPES with a spatial resolution of 4x4 µm. We demonstrate the presence of surface states and quantify the CDW gap. Our termination-resolved measurement allows us to probe the depth dependent of the Te-sheets revealing at least the presence of 3 different layer doping in a single crystal (see Fig. 1b) and explains the broad spectrums previously reported.

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A topological classification of finite chiral structures – theory and experiment

Ms M. M. McCarthy[1], Professor D. M. Whittaker[1]
[1]*University Of Sheffield, Sheffield, United Kingdom*

Topological Materials 2, June 30, 2023, 11:00 - 13:00

Coaxial cable networks are an excellent system for experiments in topological physics, because their radio frequency properties can be described using a Hamiltonian formulation, with matrix elements determined by the connections in the network. With this approach, it is easy to create networks represented by Hamiltonians with near exact chiral symmetry, and investigate their topological properties experimentally.

The use of this experimental platform presents a theoretical challenge, to determine and classify the topological phases of a finite chiral network, without the periodicity required to apply conventional momentum space methods. For a chiral structure, topological phase boundaries in the space of Hamiltonians are given by surfaces where the Hamiltonian is singular. By studying such surfaces, we propose a rigorous topological classification scheme for arbitrarily disordered finite chiral networks, and show all such structures have a classification of NZ_2, where the integer N is determined by how the structure is connected. The classification is based around determining the number of ways a structure may be fully covered by sets of disjoint pairs of connected sites. The method also predicts the number of symmetry protected topological states and enables us to analytically find phase boundaries.

We present experimental results for some simple cable networks representing graphene structures which illustrate aspects of our classification. Using a vector network analyser to measure the local density of states and transmission properties, we can determine when a structure falls on a topological phase boundary and demonstrate the existence of topologically protected states.

Anisotropic band splitting induced by applied strain to a tetragonal FeSe1-xSx

Archie Morfoot[1], Dr Tim Kim[2], Dr Matthew Watson[2], Dr Amir-Abbas Haghighirad[3], Prof Amalia Coldea[1]
[1]University of Oxford, Oxford, United Kingdom, [2]Diamond Light Source, Didcot, UK, [3]Karlsruhe Institute of Technology, Karlsruhe, Germany

Superconductivity 2, June 29, 2023, 11:00 - 13:00

The nematic order of iron-chalcogenide superconductors significantly distorts the Fermi surface due to orbital-dependent band shifts in the presence of strong electronic correlations. These effects also are momentum dependent, affecting differently the electron and hole pockets, however, the precise mechanism is not fully understood. In this work we report a detailed angle-resolved photoemission spectroscopy (ARPES) study under strain in a tetragonal FeSe1-xSx. As the selected system has a large nematic susceptibility, we can couple efficiently to the nematic order by applying in-situ strain and gradually inducing in-plane orbital anisotropy. By increasing strain, the degeneracy of the dxz and dyz bands is lifted and the energy splitting has a clear linear dependence to strain. This highlights that strain is the conjugate field to the nematic order. Surprisingly, the band shifts, although opposite in sign, differ in magnitude. We also find that, in contrast with nematic FeSe, along the tensile strain axis, two electron pockets are always resolved for FeSe1-xSx. These unexpected results may allude to a missing piece of the underlying theory, which has puzzled the community for over a decade.

Magnetic properties of the intercalated transition metal dichalcogenide Fe1/3TaS2

Dr Daniel Mayoh[1], Mr Amar Dhariwal[1], Mr Jaspal Kang[1], Prof Geetha Balakrishnan[1]
[1]*University Of Warwick, Coventry, United Kingdom*

Magnetism 3, June 30, 2023, 11:00 - 13:00

Noncentrosymmetric magnetic systems have been found to host a variety of exotic, and in some cases topologically protected, magnetic states such as skyrmion lattices, bimerons, chiral solitons and helimagnetism to list a few. One such class of material that have faced increased scrutiny in recent years for their magnetism are layered materials such as the intercalated transition metal dichalcogenides. Intercalating magnetic transition metal ions (for example, M = V, Cr, Co, Fe) into the van der Waals gap between neighboring NbS2 or TaS2 layers can lead both to a noncentrosymmetric structure and variety of complex magnetic behaviours [1,2,3,4]. Here, we report the synthesis of the chiral ferromagnet Fe1/3TaS2, by chemical vapour transport. We discuss the initial characterization of the magnetic state of Fe1/3TaS2 and compare the behaviour to other members of the intercalated transition dichalcogenides.

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Numerical simulation of Josephson traveling-wave parametric amplifier

Emil Rizvanov[1], Samuel Kern[1], Prof. Miroslav Grajcar[1,2]
[1]Department of Experimental Physics, Comenius University, Bratislava, Slovakia, [2]Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovakia

Superconductivity 2, June 29, 2023, 11:00 - 13:00

Superconducting traveling waves parametric amplifier (TWPA) is an important component in quantum sensors and quantum computers. Although standard coupled-mode theory can explain the amplification of the signal, it fails to describe complex behavior beyond the approximations utilized by the theory. To precisely predict the response of the TWPA, it is suitable to solve a system of a large number of nonlinear equations numerically. The most well-known program that allows a simulation of such systems is WRspice. This program has already been successfully used to design some amplifiers [2]. In our work, we used the new program JoSIM which uses a different numerical scheme for solving Josephson junctions circuits. We compare JoSIM [1] with WRspice in simulating the Josephson traveling-wave parametric amplifier impedance-matched to ports by tapers made of Josephson Junctions. It is shown that such a design allows for suppressing ripples in the gain profile. Both programs provide similar results, but JoSIM simulates circuits much faster than WRspice.

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Magnetic Ground States of Non-linear Antiferromagnetic Coordination Polymer Chains

Shroya Vaidya[1], Dr. Roger Johnson[2], Dr Jamie Manson[3], Dr John Singleton[4], Dr. Paul Goddard[1]
[1]University of Warwick, Coventry, United Kingdom, [2]University College London, London, United Kingdom, [3]Eastern Washington University, Washington, United States of America, [4]National High Magnetic Field Laboratory, Los Alamos, United States of America

Magnetism 4, June 30, 2023, 15:00 - 17:00

Coordination polymers, in which lattices of magnetic metal ions are bridged by ligands, have proven to be an effective platform for exploring the properties of low-dimensional quantum magnets [1]. The ability to interchange the ligand species make these systems highly tuneable. Additionally, organic ligands such as pyrimidine (pym) allows the study of non-linear chain structures, which are not easy to realise in entirely inorganic structures. Previously, pym has been used to synthesise the staggered and chiral Cu(II) spin-1/2 antiferromagnetic chains, pym-Cu(NO3)2(H2O)2 [2] and [Cu(pym)(H2O)4]SiF6·H2O [3], respectively.
In these materials, the alternating orientation of the local spin environment gives rise to non-trivial staggered g tensors and Dzyaloshinskii-Moriya (DM) interactions which, on application of an external magnetic field, generate a staggered field and an unusual field-dependent energy gap [4]. In a theoretical tour de force it was shown that mapping the Hamiltonian to the sine-Gordon quantum-field theory accounts for this behavior in the staggered chain [5,6]. However, similar physics remains to be fully explained for the chiral chain.

Recently, we synthesized the spin-1 Ni(II) analogues, Ni(pym)(NO3)2(H2O)2 and [Ni(pym)(H2O)4]SO4, of the staggered and chiral chains, in addition to third a non-linear structure NiCl2(pym)2. In these systems, an alternating single-ion anisotropy axis is expected to accompany the alternating local g tensors. We have used muon spin rotation and high field magnetisation experiment to infer the magnetic properties of these materials. Here, we present the ordered magnetic structure resulting from the competition of the exchange and unusual alternating anisotropy axis.

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Evaluating and optimising proximity-induced magnetism in MnTe/Bi2Te3 heterostructures

Geet Awana[1], Ryuji Fujita[2], Andreas Frisk[3], P. Chen[4], Q. Yao[4], A. J. Caruana[5], C. J. Kinane[5], N.-J. Steinke[6], Sean Langridge[5], P. Olalde-Velasco[3], S. S. Dhesi[3], Gerrit van der Laan[3], X. F. Kuo[4], S. L. Zhang[4], Thorsten Hesjedal[2], **Dirk Backes[3]**

[1]Loughborough University, Loughborough, United Kingdom, [2]University of Oxford, Oxford, United Kingdome, [3]Diamond Light Source, Didcot, United Kingdom, [4]ShanghaiTech University, Shanghai, United Kingdom, [5]ISIS Muon & Neutron Source, Oxon, United Kingdom, [6]Institute Laue-Langevin, Grenoble, France

Topological Materials 1, June 29, 2023, 11:00 - 13:00

The introduction of magnetism in topological insulators, semiconducting materials that are non-magnetic by nature, has long been sought after to realise exotic quantum effects. Most prominent is the quantum anomalous Hall effect (QAHE), where electronic surface states can propagate dissipationless through a material [1]. Additionally, these states are 100% spin-polarised and immune to external perturbations, rendering them ideal candidates for spintronics applications as well as for new concepts for quantum computing.

The QAHE is not restricted to a particular temperature range but has so far only been observed at around 1 K in magnetically doped topological insulators [2]. Thus, the task at hand is to find new concepts to magnetise the topological insulator. Here, we investigate a new approach based on proximity induced magnetisation in heterostructures, where the topological insulator Bi_2Te_3 and the topologically trivial, magnetic add-layer MnTe share an interface but are otherwise spatially separated [3]. We employ polarised neutron reflectivity, polarised x-ray spectroscopy and magnetotransport measurements to evaluate the magnetic properties of each individual layer and the magnetic landscape at the MnTe /Bi_2Te_3 interface. We find the MnTe layer in a ferromagnetic instead of the anticipated antiferromagnetic state and that Mn constituents penetrate into the Bi_2Te_3 layer. Those effects go often unnoticed and can be misinterpreted as proximity induced magnetisation, for which no indication can be found. We provide a robust, multitechnique approach to gain a complete picture of the magnetisation and to optimise the interface, and thereby increasing the temperature range the QAHE can be observed. Our work thus contributes to the transformation of magnetic topological insulators from fundamental research to practical applications.

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Hierarchy of Lifshitz transitions in the surface electronic structure of Sr2RuO4 under uniaxial compression

Edgar Abarca Morales[2], Gesa-R. Siemann[1], Andela Zivanovic[1,2], Philip A. E. Murgatroyd[1], Igor Marković[1,2], Brendan Edwards[1], **Chris Hooley[1]**, Dmitry A. Sokolov[2], Naoki Kikugawa[3], Cephise Cacho[4], Matthew D. Watson[4], Timur K. Kim[4], Clifford W. Hicks[2,5], Andrew P. Mackenzie[1,2], Phil D. C. King[1]
[1]SUPA, University Of St Andrews, St Andrews, United Kingdom, [2]Max Planck Institute for the Chemical Physics of Solids, Dresden, Germany, [3]National Institute for Materials Science, Tsukuba, Japan, [4]Diamond Light Source, Harwell Science and Innovation Campus, Didcot, United Kingdom, [5]School of Physics and Astronomy, University of Birmingham, Birmingham, United Kingdom

Surfaces, Interfaces and Thin Films, June 30, 2023, 11:00 - 13:00

Many of the listed co-authors of this abstract recently carried out an experimental study [1] of the evolution of the electronic structure at the surface of the layered perovskite Sr2RuO4 under large in-plane uniaxial compression. They demonstrated the existence of a sequence of Lifshitz transitions, which reshape the low-energy electronic structure and the rich spectrum of van Hove singularities that the surface layer of Sr2RuO4 hosts. In this talk, I present tight-binding modelling, principally carried out by Edgar Abarca Morales [1], which demonstrates that - somewhat surprisingly - the strain is accommodated predominantly by bond-length changes rather than by modifications of octahedral tilt and rotation angles. I discuss the suggestion that this preference for bond-length changes rather than rigid-octahedron-type distortions may actually be intimately related to the electronic structure changes mentioned above.

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Multi-Q magnetic phases from frustration and chiral interactions

Marios Georgiou[1], Ioannis Rousochatzakis[1], Joseph Betouras[1]
[1]*Loughborough University, Loughborough, United Kingdom*

Magnetism 2, June 30, 2023, 09:30 - 10:30

We investigate the effect of Dzyaloshinskii-Moriya (DM) interactions in the planar pyrochlore (checkerboard) antiferromagnet, one of the paradigmatic models of spin frustration, and establish the classical phase diagram using a combination of analytical and numerical approaches. While anisotropic interactions generally tend to remove the frustration, here we show that a high degree of frustration survives in a large region of the phase diagram. In conjunction with the fixed handedness introduced by the DM anisotropy, this spawns a cascade of incommensurate and double-twisted multi-domain phases, consisting of spatially intertwined domains of the underlying competing phases of the isotropic frustrated point. The results underpin a novel mechanism of generating multi-Q phases in systems that combine high degree of frustration and chiral interactions.

Supercurrent-enabled Andreev reflection in a chiral quantum Hall edge state

Bernd Braunecker[1]
[1]*University of St Andrews, St Andrews, United Kingdom*

Superconductivity 2, June 29, 2023, 11:00 - 13:00

We discuss how a chiral integer quantum Hall edge (QHE) state placed in proximity to an s-wave superconductor can experience induced superconducting correlations [1]. In a QHE the superconducting proximity effect faces the obstacle that the Cooper pairs of the superconductor are spin singlets with zero centre-of-mass momentum, whereas the quantum Hall edge is spin polarised and chiral, thus all particles are moving in the same direction. One would hence expect it to be hard to induce superconducting pairing in a quantum Hall edge, yet recent experiments have shown this to be possible [2]. We present a microscopic theory showing how induced superconducting pairing becomes possible through the combination of spin-orbit interaction in the interface region together with the supercurrent arising from the Meissner effect. By integrating out the degrees of freedom of the s-wave superconductor we obtain an effective pairing Hamiltonian in the QHE state. We clarify the qualitative appearance of nonlocal superconducting correlations in a chiral edge state and analytically predict the suppression of electron-hole conversion at low energies (Pauli blocking) and negative resistance as experimental signatures of Andreev reflection in this setup. We furthermore discuss that the induced pairing state has unusual topological properties.

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Flat bands, localised states, and non-trivial topology of one-dimensional Lieb superlattices

Mr Dylan Jones[1], Adelina Ilie[1], Lucian Covaci[2]
[1]*University Of Bath, Bath, United Kingdom,* [2]*University of Antwerp, Antwerp, Belgium*

Topological Materials 1, June 29, 2023, 11:00 - 13:00

Systems possessing electronic flat bands have interested researchers as a platform for investigating strongly correlated phenomena. The Lieb lattice is one system that contains a flat band, in addition to topological edge states and a non-trivial quantum geometry, a key ingredient for realising topological superconductivity [1]. But this flat band disperses upon inclusion of second nearest-neighbour electron hoppings, which are unavoidable in realistic solid-state systems due to the finite decay length of the electron wavefunctions. Application of a 1D periodic potential to graphene can induce band flattening, but analytical electronic dispersion calculations for a 1D Lieb superlattice do not predict a similar effect [2]. However, this calculation builds the dispersion relation from the low-energy eigenstates of the pristine lattice, preventing determination of a full band structure and prohibiting the resolution of highly localised flat band states and other features that result from lattice symmetry breaking.

To fully study the electronic states of a 1D Lieb superlattice, the Hamiltonian must be solved numerically. We do this in a single-particle tight-binding framework, utilising Exact Diagonalisation and Kernel Polynomial functionalities of the open-source Pybinding package [3]. We consider short and long periodicities; tilted cones are observed in the former case and highly degenerate flat band states, which manifest as van Hove singularities, emerge for increasing superlattice periodicities. For long periodicities we compare the electronic dispersion to that obtained with the continuum model, revealing the effects of lattice symmetry breaking and charge-carrier localisation, which are not resolved analytically, on the density of states and conductivity. We also show that modifications to localisation behaviour can be introduced by smoothing the potential and demonstrate the effect on the above observables. Finally, we show that non-trivial topological edge states which couple to the system's flat bands can be realised through tuning of the lattice Hamiltonian parameters.

Our results demonstrate the suitability of 1D Lieb superlattices as hosts of exotic electronic states due to the presence of tilted Dirac cones and highly degenerate flat bands for short and long periodicities. The prediction of a topological edge state that couples to the system’s flat bands makes this system a candidate for realising topological superconductivity, with potential applications in fault-tolerant quantum computing. Future studies that include the effects of disorder and interactions will be crucial in elucidating the exact nature of the strongly correlated states in this system.

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Fermi surfaces and quasiparticle effective masses in the high-pressure phase of superconducting iron-chalcogenides, FeSe1-xSx

Amalia Coldea[1]
[1]*University of Oxford, Oxford, United Kingdom*

Superconductivity 2, June 29, 2023, 11:00 - 13:00

Electronic nematic and spin-density wave phases of FeSe family of iron-chalcogenides superconductors can be intertwined and difficult to assess their relevance on superconductivity. Tuning parameters, like applied pressure and chemical pressure [1,2], can be used to explore their relative importance. Here, I will present quantum oscillations studies under high applied hydrostatic pressure in FeSe1-xSx using magnetotransport and tunnel diode oscillator experiments [3,4,5]. I will discuss the evolution of the Fermi surface and electronic correlations inside the high-pressure phase where superconductivity is enhanced. Our findings emphasize the robustness of the high-pressure superconducting phase, despite the fragility of other competing electronic phases to different conditions [5,6].

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Phase transition and Moiré superlattices in the two-dimensional single and few-layer NiI2 transition metal dihalide

Liam Turnpenny[1], Esyllt Williams[1], Kei Takashina[1], Adelina Ilie[1]
[1]*University of Bath, Bath, United Kingdom*

Helium and Complex Structured Materials, June 29, 2023, 11:00 - 13:00

Multiferroic magnetoelectric 2D semiconducting materials are at the core of new concepts of spintronic devices that aim to control magnetism with an electric field, while being able to concurrently modulate carrier density. NiI2 is one of just a few exemplars of this class of 2D materials. Chemical vapour deposition (CVD)-grown NiI2 has been recently demonstrated by optical techniques to be multiferroic, i.e. with co-existing and interlinked magnetisation and ferroelectric order-down to the monolayer (with Tc ~21K)[1]. Monolayer NiI2 was also predicted to be ferromagnetic (FM) below 170 K, one of the highest Curie temperatures for a semiconductor[2].

We synthesized NiI2 by molecular beam epitaxy (MBE) for the first time, in UHV and on Au(111) and studied it primarily with Scanning Tunneling Microscopy/Spectroscopy and variants. Our synthesis process led to monolayer NiI2 growing on “buffer” layers that decouple NiI2 from the Au(111) substrate, leading to a complex, unique system that is very different to those grown by CVD. Acharacteristic, unusual Moiré superlattice predominantly forms, that is distinct from the normal superlattices obtained by 2D materials with their substrates: it is not a simple hexagonal superlattice, but a(√3×√3)R30°of a primary Moiré. Moreover, 1D superlatticesare also observed in the minority.

Our scanning tunneling spectroscopy (STS) data at 77 and 4 K demonstrates that a phase transition occurs between the two temperatures(Fig. a). The (√3×√3) R30°superlattice modulates the spin-polarised, energy-confined states seen above the Fermi energy (Fig. b) and is expected to generate spin texture (as supported byDFT simulations on our material); a different spin texture is expected to arise from the 1D superlattice. We explain the origin of these 2D and 1D superlattices and link them to the nature of the subsurface layers. We also investigate the local and non-local effect of an electric field. All these shed light on the magnetoelectric properties of this complex multi-layered system.

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Exact Results on the Anomalous Hall Effect in the Dirac Semimetal ZrTe5

Gabriel Cardoso[1]

[1]*Tsung-Dao Lee Institute, Shanghai Jiao Tong University, Shanghai, China*

Topological Materials 1, June 29, 2023, 11:00 - 13:00

Measurements of the anomalous Hall effect (AHE) provide a good probe into the topology of the band structure of Dirac semimetals. We consider the interesting material $ZrTe_5$ and show how the AHE's temperature and magnetic field dependence can be explained in terms of a temperature-induced Lifshitz transition and a magnetic field-induced nodal line formation. In our calculation, we adopt a k.p model of the Dirac cone and compute the Hall conductivity analytically, even in the high-magnetic field regime where Landau levels are formed. Surprisingly, the exact, fully quantum result can be replicated by a semi-classical prescription in radial gauge. Finally, a careful comparison of the results with experimental data points towards the emergence of a temperature-induced topological phase transition.

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Separation of heating and magneto-elastic coupling effects in surface acoustic wave-enhanced magnetic domain wall creep motion

Dr Thomas Moore[1], **Mr Jintao Shuai[1]**, Mr Robbie Hunt[1], Professor John Cunningham[1]
[1]*University Of Leeds, Leeds, United Kingdom*

Magnetism 3, June 30, 2023, 11:00 - 13:00

Surface acoustic waves (SAWs) show significant potential for energy-efficient control of magnetic domain wall (DW) creep motion owing to the magneto-elastic coupling effect [1]. However, the SAW-induced heating can also contribute to the DW motion [2]. In this work, the heating of a SAW device was measured locally using an on-chip Pt film as a thermometer within the SAW beampath. Fig.1 shows the diagram of the devices. Two interdigitated transducers (IDTs), whose centre frequency is 48 MHz, were patterned on opposite ends of a 2-mm-wide stripe of Ta(5.0)/Pt(2.5)/Co(0.9)/Ta(5.0) thin film (thicknesses in nm). The film was prepared by dc magnetron sputtering onto a lithium niobate substrate, which can support the propagation of SAWs. Results show that a temperature increase of ~10 K was observed within the SAW beampath with the application of SAWs at the centre frequency of 48 MHz and a total RF power of 21 dBm (Fig. 2a). DW velocity was also measured using Kerr microscopy at various temperatures or in the presence of SAWs (Fig. 2b). With a 10 K increase in temperature and no SAWs applied, DW velocity increases from 33±3 μm/s (at room temperature) to 104±8 μm/s at an external magnetic field of 65 Oe. Travelling SAW-assisted DW velocity (116±3 μm/s) is slightly higher than that with a 10 K temperature increase suggesting that heating plays the major role in promoting DW motion, whereas the DW motion is significantly enhanced (418±8 μm/s) in the presence of standing SAWs suggesting that magneto-elastic coupling effect is more important than heating in this case [3].

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QUEST-DMC: Superfluid Helium-3 Bolometers for a Direct Dark Matter Search

Miss Tineke Salmon[1,3], Dr Samuli Autti[1,3], Dr Neda Darvishi[2,3], Dr Paolo Franchini[1,2,3], Professor Richard Haley[1,3], Dr Ashlea Kemp[2,3], Dr Elizabeth Leason[2,3], Dr Lev Levitin[2,3], Professor Jocelyn Monroe[2,3], Mr Robert Smith[2,3], Professor Stephen West[2,3], Dr Vladislav Zavyalov[1,3], Dr Dmitry Zmeev[1,3]
[1]Lancaster University, Lancaster, United Kingdom, [2]Royal Holloway University of London, Egham, United Kingdom, [3]QUEST-DMC Collaboration,

Helium and Complex Structured Materials, June 29, 2023, 11:00 - 13:00

The QUEST-DMC collaboration is conducting a direct dark matter search using superfluid helium-3 as a target. Dark matter is inferred from gravitational lensing, galaxy rotation curves, cosmic microwave background, and a bullet cluster, as it does not interact with electromagnetic fields. The goal of the experiment is to detect spin-dependent interactions in the sub-GeV mass range as heat deposited in the superfluid in the eV range.

To achieve this, the He-3 is cooled down to 100 μK, where broken Cooper pairs generate thermal excitations with energy 10^(-7) eV. By moving a probe rod in the superfluid and measuring changes in the drag force, energy deposited by a dark matter collision can be detected. Simulations of background events and nuclear and electron recoil energies have been conducted. To ensure the radiopurity of the experiment and to facilitate the correct interpretation of the background signal, radioassays have been completed.

The He-3 target is contained in a bolometer box, which has been calibrated using the width parameter response of a wire resonator after injecting heat. Ongoing work includes calibrating the bolometers for energy deposits and incorporating photon detection as a secondary signal. Additionally, a SQUID is being tested as a less noisy alternative to the direct readout of the wires used presently. Here we discuss the preliminary results of the collaboration such as the bolometer calibration. This abstract was written on behalf of the QUEST-DMC Collaboration.

Dynamics of the critical phonon modes in quantum paraelectric $SrTiO_3$

Shiyu Deng[1], Dr. Charles R. S. Haines[1,2], Dr. David M. Jarvis[1,3], Dr. Matthew J. Coak[1,4], Dr. Alexandre Ivanov[3], Dr. Andrea Piovano[3], Dr. Andrew R. Wildes[3], Dr. Siddharth S. Saxena[1]
[1]University of Cambridge, Cambridge, United Kingdom, [2]University of East Anglia, Norwich, United Kingdom, [3]Institut Laue-Langevin, Grenoble, France, [4]University College London, London, United Kingdom

Metals and Correlated Electron Systems 1, June 29, 2023, 09:30 - 10:30

The proximity of $SrTiO_3$ to a ferroelectric quantum critical point (FE QCP) has become a promising new branch of the study of quantum critical phenomena. New forms of quantum order have been reported in $SrTiO_3$ different from the quantum paraelectric state via dielectric measurements [1-3]. The critical point here is associated with a soft optical phonon mode responsible for the ferroelectric instability.

We report our recently performed triple-axis inelastic neutron scattering experiments on single-crystal $SrTiO_3$ at the temperature and pressure region of interest. These were the first direct measurements deep into the enigmatic "quantum polar-acoustic state" in the vicinity of the FE QCP. Measurements are taken at and around q = 0 in multiple directions in reciprocal space to explore the transverse acoustic and soft optical phonon modes and their hybridization. In addition, we explore how pressure affects the underlying phonon modes in $SrTiO_3$. Our observations directly address the coupling of the soft optical mode with the acoustic phonons and its response to external pressure. We believe this could help us understand the importance of anharmonic lattice dynamics and quantum fluctuations in $SrTiO_3$.

* This work is supported by Cavendish Laboratory and Jesus College, Cambridge, and the Department of Business, Energy and Industrial Strategy, UK (BEIS Grant Number: G115693). The experiments were carried out with the support of the Institut Laue-Langevin, Grenoble, France through the approval of beamtime for proposals 7-02-212, 7-02-213 and 7-02-219.

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4He and 3He – 4He mixture films studied by neutron reflectometry.

Dr Oleg Kirichek[1], Dr Chris Lawson[1], Dr Christy Kinane[1], Dr Andrew Caruana[1], Dr Timothy Charlton[2], Prof Sean Langridge[1], Prof Peter McClintock[3]
[1]ISIS Faility, STFC, UKRI, Didcot, United Kingdom, [2]Oak Ridge National Lab, Oak Ridge, USA, [3]Lancaster University, Lancaster, United Kingdom

Helium and Complex Structured Materials, June 29, 2023, 11:00 - 13:00

Of the many quantum fluid systems superfluid helium films remain one of the most elusive for experimental investigation. We used neutron reflectometry to study liquid 4He and 0.1% 3He in 4He mixture films. Thanks to the exceptional sensitivity and precision of this technique, we could observe and study 165 Å thick superfluid helium film formed on a silicon surface in temperature range from 170 mK to 1.5 K. In the temperature range of the experiment the change in reflectivity signal from 4He film is insignificant. Addition of 0.1% of 3He dramatically changes the film behavior. In the helium mixture film almost all adsorption comes from neutron scattering on 3He atoms, therefore neutron adsorption part of scattering length represents distribution of 3He atoms inside the film. At lowest temperature of 170 mK we observe a phase-separated 3He -4He mixture film with 3He situated close to the surface. With the temperature increasing we witness a gradual dissolution of its 3He top layer into 4He. At around 300 mK whole helium film almost vanishes from the surface of the silicon substrate, leaving just clusters of mostly 3He atoms. The observed anomaly in the film behavior may be associated with phase transition. In the experiment we also found out an unexpected restoration of the layered structure at 1.5 K. Our results could be important for development of the powerful dilution refrigerators which, to significant extent, are limited by film flow effects.

An ab initio Study of Electron Transport in Ultra-Wide Band Gap Semiconductors

Patrick Williams[1], Dr Angela Dyson[1], Prof. Patrick Briddon[1]
[1]*Newcastle University, Newcastle Upon Tyne, United Kingdom*

Semiconductors, June 29, 2023, 09:30 - 10:30

With the advent of electric vehicles and the phasing out of fossil fuels, more strain will be placed on the electrical power sector where most power devices are Si based. Si has reached the limit of what it is capable of in these applications and interest has turned to wide bandgap semiconductors which show promise in making power devices with smaller form factors and higher operating efficiency [1,2]. Furthermore, there has been an increase in interest in ultra-wide band gap (UWBG) semiconductors beyond power electronics due to their emission of light in deep UV, thermal stability and radiation hardness [3,4,5].

However, due to the nascent stage of development of UWBG semiconductors, much remains unknown about their properties and there is a lack of device simulation models resulting in estimations of experimental parameters [6, 7]. A promising avenue of research, therefore, is the use of ab initio studies to predict unknown parameters for use in Monte Carlo (MC) simulation of electron transport. Here, we present the results of an investigation into the electron transport of two UWBG semiconductors of interest, diamond and cubic-BN; with Si as a benchmark. Specifically, the density of state and parameters of interest are extracted from density functional theory using a non-uniform tetrahedral grid, which are then used for the calculation of scattering tables in MC simulation to show agreement with analytic simulators as a first step in developing new tools for the simulation of the next generation of devices.

Fig. 1. A comparison of the average drift velocity vs field for GaAs (purple), Si (blue), GaN (green), diamond (red) and cubic BN (orange) generated using analytic MC simulator.

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Site-controlled InAs/GaAs Quantum Dot arrays for nanophotonics

Chak Lam Chan[1], Dr. Aris Trapalis[1], Dr. Charlotte Ovenden[1], Dr Ian Farrer[1], Dr Dominic Hallet[2], Dr Ed Clarke[3], Professor Maurice Skolnick[2], Professor Jon Heffernan[1,3]
[1]University of Sheffield, Department of Electronic and Electrical Engineering, Sheffield, United Kingdom, [2]University of Sheffield, Department of Physics and Astronomy, Sheffield, United Kingdon, [3]National Epitaxy Facility, Sheffield, United Kingdom

Semiconductors, June 29, 2023, 09:30 - 10:30

Controlling the position of quantum dots (QDs) is desirable for nanophotonic devices due to their potential as single photon emitters for quantum technology applications.1 Challenges that are associated with forming site controlled QDs include single QD occupation, planarisation, low linewidth and controllable wavelength. For Stranski-Krastonov growth, QDs nucleate preferentially in local minima in the surface chemical potential.2 In this study, we use ex-situ fabrication of arrays of nanoholes to form these preferential nucleation sites. We investigated the effects of nanohole size, nanohole density and other parameters on emission wavelength of single QDs.

Initial development focused on good site-selectivity of QD arrays, which allowed for optimisation of growth parameters to control emission wavelength and QD linewidth. Planarisation on the patterned surface was also crucial: during the GaAs buffer layer preservation of the nanoholes is important to allow them to function as preferential nucleation sites, but after QD formation planarisation of the capping layer is important for good optical properties, for example in waveguides. These conditions resulted in nucleated QDs with a minimum linewidth of 22μeV (resolution limited) and an average linewidth ~87μeV measured using non-resonant excitation.

Each sample contains different arrays with variation in nanohole size and density, allowing for direct investigation of the effects of these parameters on the emission wavelength and linewidth of nucleated quantum dots using site-specific photoluminescence (PL) measurements. We observe shifting of emissions in the range of 900 to 1000nm, compatible with high-efficiency Si detectors. From micro-PL measurements, clusters of uniform single line emissions are obtained.

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Numerical simulations of spin dynamics using a path integral method

Dr Thomas Nussle[1], Dr Stam Nicolis[2], Dr Joseph Barker[1]
[1]School of Physics and Astronomy, University of Leeds, Leeds, United Kingdom, [2]Institut Denis Poisson, Université de Tours, Université d'Orléans, CNRS (UMR7013), Tours, France

Magnetism 3, June 30, 2023, 11:00 - 13:00

A common way to study finite temperature effects in condensed matter physics is to introduce a thermal noise into the equations of motion, thus promoting these to stochastic equations. One then solves these equations for several different realisations of the noise and averages over these solutions to yield the moments of the statistical distribution of the relevant degrees of freedom. In molecular dynamics, where the relevant degrees of freedom are positions and momenta of particles, this leads to a pictorial representation of temperature as fluctuations around a given equilibrium. Going to lower and lower temperatures, this leads to a fundamental contradiction, namely simultaneous computation of position and momenta to arbitrary precision, which breaks the Heisenberg uncertainty principle. It is, however, possible to recover an effective classical model which yields the correct quantum expectation values by using path integrals, without simulating the full quantum system. Such methods are known as Path Integral Molecular Dynamics.

Inspired by these methods, we propose a similar approach for a spin in a magnetic field, which while resulting in a classical model, accounts for effects due to the underlying spin quantisation. We start by expressing the spin algebra in the spin coherent states basis, thus enabling the transition from a discrete to a continuous quantum description. We then rewrite its quantum mechanics in the framework of Path Integrals, hence yielding a partition function as an integral rather than a sum. We approximate the resulting partition function in the high-temperature limit by recasting the quantum matrix elements into an effective exponential form hence deriving an effective, equivalent, classical Hamiltonian. In this form, the quantised nature of spin takes the form of effective anisotropy terms added to standard coupling to the applied field. We then proceed to solve this effective classical model by implementing an effective field derived from this classical, effective, Hamiltonian into an atomistic spin dynamics model from which we derive thermodynamic observables and show that our effective model produces accurate quantum expectation values within its relevant temperature range.

High performance rapid turn-around cryogen-free microkelvin platform: unlocking the sub-1mK temperature range for quantum materials research

Dr Ján Nyéki[1], Dr Marijn Lucas[1,3], Mrs Petra Knappová[1], Dr Lev Levitin[1], Dr Andrew Casey[1], Professor John Saunders[1], Dr Harriet van der Vliet[2], Dr Anthony Matthews[2]
[1]Royal Holloway, University of London, Egham, TW20 0EX, United Kingdom, [2]Oxford Instruments NanoScience, Tubney Woods, Abingdon, OX13 5QX,, United Kingdom, [3]University of Delft, , Netherlands

1. Nonequilibrium Physics 2. Instruments and Applications, June 30, 2023, 15:00 - 17:00

Improved accessibility to the microkelvin temperature regime is important for future research in quantum materials; quantum information science; applications of quantum sensors. Here we report the design and performance of a microkelvin platform based on a nuclear demagnetization stage, engineered, and optimized for operation on a standard cryogen-free dilution refrigerator [1]. $PrNi_5$ is used as the dominant refrigerant. The platform has a large area for mounting experiments in an ultralow temperature, low electromagnetic noise environment.

We demonstrate cooling to 395 µK. We have established a mode of operation, with a duty cycle in which we remain below 1mK for 95% of the time.

The platform has already provided an efficient cryogen-free microkelvin environment for the exploration of frontier science and technology on a range of systems. We highlight several collaborative experiments enabled by the European Microkelvin Platform.

The research leading to these results has received funding from the European Union's Horizon 2020 Research and Innovation Programme, under Grant Agreement no. 824109.

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Interplay of Hidden Orbital Order and Superconductivity in CeCoIn5

Weijiong Chen[1], Clara Neerup Breiø[2], Freek Massee[3], Milan Allan[4], Cedomir Petrovic[5], Séamus Davis[1,6,7,8], Peter Hirschfeld[9], Brian Andersen[2], Andreas Kreisel[2,10]

[1]Clarendon Laboratory, University of Oxford, Oxford, United Kingdom, [2]Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark, [3]Laboratoire de Physique des Solides Bâtiment 510, Université Paris-Sud, Orsay, France, [4]Leiden Institute of Physics, Leiden University, Leiden, The Netherlands, [5]CMPMS Department, Brookhaven National Laboratory, Upton, USA, [6]LASSP, Department of Physics, Cornell University, Ithaca, USA, [7]Department of Physics, University College Cork, Cork, Ireland, [8]Max-Planck Institute for Chemical Physics of Solids, Dresden, Germany, [9]Department of Physics, University of Florida, Gainesville, USA, [10]Inst. für Theoretische Physik, Universität Leipzig, , Germany

Superconductivity 3, June 30, 2023, 15:00 - 17:00

Visualizing atomic-orbital degrees of freedom is a frontier challenge in scanned microscopy. Some types of orbital order are virtually imperceptible for normal scattering technique because they do not reduce the overall crystal lattice symmetry. A good example is dxz/dyz (π,π) orbital order in tetragonal lattices. For enhanced detectability, here we consider the quasiparticle scattering interference (QPI) signature of such (π,π) orbital order in both normal and superconducting phases. The theory reveals that sublattice-specific QPI signatures generated by the orbital order should emerge strongly in the superconducting phase. Sublattice-resolved QPI visualization in superconducting CeCoIn5 then reveals two orthogonal QPI patterns at lattice-substitutional impurity atoms. We analyze the energy dependence of these two orthogonal QPI patterns and find the intensity peaked near E=0, as predicted when such (π,π) orbital order is intertwined with d-wave superconductivity. Sublattice-resolved superconductive QPI techniques thus represent a new approach for study of hidden orbital order.

Topological superfluid helium-3 under mesoscopic confinement

Dr Petri Heikkinen[1], Dr Lev Levitin[1], Dr Andrew Casey[1], Dr Xavier Rojas[1], Dr Angadjit Singh[1], Mr Nathan Eng[1], Dr Anton Vorontsov[2], Dr Priya Sharma[1], Dr Nikolay Zhelev[3], Dr Thanniyil Abhilash[3], Prof Jeevak Parpia[3], Prof John Saunders[1]

[1]Royal Holloway, University Of London, Egham, United Kingdom, [2]Montana State University, Bozeman, USA, [3]Cornell University, Ithaca, USA

Helium and Complex Structured Materials, June 29, 2023, 11:00 - 13:00

The firmly established unconventional spin-triplet p-wave nature of superfluidity in helium-3 allows using its various superfluid phases as benchmark systems for topological superconductivity. Under strong confinement, anisotropic surface pair-breaking dominates the superfluid properties, favouring chiral ^{3}He-A phase over time-reversal-invariant ^{3}He-B phase. Prior experimental extremely sensitive SQUID-NMR studies of ^{3}He in nanofabricated slab-shaped cavities of height D comparable to the size of the Cooper pairs ξ_o, tuneable between 20 and 80 nm by pressure, have demonstrated the influence of confinement on the superfluid order parameter [1,2], including evidence for a spatially modulated pair-density wave [3] and survival of ^{3}He-A down to the quasi-2D limit $D/\xi_o = 1$ [4]. Since ^{3}He is an extremely pure and defect-free system, and thus is not affected by impurity-related pair breaking, we can experimentally access the pure surface-and-edge-related effects such as the suppression of order parameter and the connected existence of topologically protected surface-bound-states (SBS) which are predicted to be of Majorana character. Quasiparticle scattering boundary condition other than specular on the surfaces results in an additional pair breaking and generation of an excess of non-topological SBS. Thus, it is important we can tune the boundary condition in situ away from the most-suppressing magnetically active solid ^{3}He layer towards diffuse and specular boundaries via addition of controlled amount of ^{4}He impurities coating all the sample surfaces with ^{4}He film [5]. Here we will describe our current and future experimental efforts to harness low magnetic fields, confinement towards the 2D limit, and hybrid multi-height cavities for sculpture of mesoscopic ^{3}He superfluid, including experiments on cosmologically relevant phase transitions in isolated volumes and thermal (Hall) transport in confined volumes and across phase boundaries.

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Magnetoelectric coupling of Terbium Tantalate

Xiaotian Zhang[1], Dr Nicola Kelly[2], Dr Denis Cheptiakov[3], Miss Shiyu Deng[1], Mr Cheng Liu[1], Prof Sian Dutton[1], Dr Siddharth Saxena[1]

[1]University of Cambridge, Cambridge, United Kingdom, [2]University of Oxford, Oxford, United Kingdom, [3]Paul Scherrer Institute, Villigen, Switzerland

Magnetism 4, June 30, 2023, 15:00 - 17:00

Quantum magnetoelectric materials form a new and emerging area of physics where one expects to find the emergence of novel quantum phases induced by subtle coupling between spin and charge degrees of freedom at low temperatures [1-2]. Experimental study of such phenomena is limited by the lack of model materials where magnetism and dielectric properties can be tuned using magnetic fields at low temperatures. In a recent breakthrough, we found that M-TbTaO4 exhibits enhancement in dielectric response below its Néel temperature on the application of a magnetic field, indicating a coupling effect between spin order and charge order. Powder neutron diffraction (PND) was used to solve the magnetic structures and atomic distances at different fields. The magnetic Tb3+ ions form a distorted diamond structure [3] (Figure 1) which could be stretched by applying a magnetic field, potentially explaining the magnetoelectric coupling.

Figure 2 shows the temperature dependence of the relative dielectric constant for M-TbTaO4 under several magnetic fields. With an increasing magnetic field, low-temperature dielectric constants gradually increase and finally, an upturn is observed below its Néel temperature. This enhancement in dielectric behavior below TN indicates a potential coupling effect between the spin order and charge order. The interatomic distance was also obtained from the refined PND data. From 0 to 6 T, there is a slight increase in d2 but a decrease in d1 for Tb ions. The stretching mechanism due to the atomic displacement under a magnetic field may explain the magnetoelectronic coupling effect.

Electron skew scattering by ferroelastically frustrated magnetic spins

Wei Peng[1,2,3], Wenjie Meng[4], Richard Beanland[1], Marin Alexe[1], Qingyou Lu[4], Tae Won Noh[2,3]
[1]Department of Physics, University Of Warwick, Coventry, United Kingdom, [2]Center for Correlated Electron Systems, Seoul National University, Seoul, Republic of Korea, [3]Department of Physics and Astronomy, Seoul National University, Seoul, Republic of Korea, [4]High Magnetic Field Laboratory, Chinese Academy of Sciences and University of Science and Technology of China, Hefei, China

Magnetism 3, June 30, 2023, 11:00 - 13:00

Multiferroics offer a fertile ground for exploring emergent phenomena and multifunctionality. While ferroelasticity – defined by an elastic hysteresis from switching between multiple orientation states under mechanical stress – widely coexists with other ferroic properties, the interplay of magnetism with ferroelasticity has received far less attention. Here we show that artificially-designed ferroelastic domains in a ferromagnetic metal, namely $SrRuO_3$, can generate a large, unconventional anomalous Hall resistance. Via microscopic characterizations, we show robust magnetic inhomogeneity that is coupled to the ferroelastic domains. We suggest that spatial evolution of structural order parameters along with built-in strain fields across the ferroelastic domain walls could frustrate the magnetic ordering and induce non-coplanar spin textures. The noncoplanar spin cluster with scalar spin chirality is supposed to deflect the motion of electrons via skew scattering, as generally limited to chiral and frustrated magnetic systems. Our results suggest great potential of spin texture engineering via coupled ferroelasticity for future spintronics.

The 3d-5d exchange interactions and orbital hybridization in Ba- and Ca-doped La2CoIrO6 double perovskite

Jose Renato Linares Mardegan[4], **Larissa Ishibe Veiga[1]**, T. Pohlmann[4], D. S. Dhesi[1], S. Francoual[4], J. R. Jesus[3], C. Macchiutti[3], E. M. Bittar[3], L. Bufaical[2]
[1]Diamond Light Source, Didcot, United Kingdom, [2]Instituto de Fisica, Universidade Federal de Goias, Goiania, Brazil, [3]Centro Brasileiro de Pesquisas Fisicas, Rio de Janeiro, Brazil, [4]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

Metals and Correlated Electron Systems 3, June 30, 2023, 09:30 - 10:30

Ir-based oxides have been extensively investigated mainly due to their extended 5d orbitals, which gives rise to a unique interplay between the strong spin-orbit coupling (SOC), the Coulomb repulsion and the crystal field splitting. In particular, the double perovskite (DP) systems, which combine Ir and 3d transition-metal ions, have led to many interesting phenomena. In this context, using Co ion as the 3d TM to interact with the neighbour's 5d TM adds further complexity to the stabilization of magnetism in these Ir-based DPs. The delicate balance between crystal field and interatomic exchange interactions can lead to different valences and spin states of the Co ions in the octahedral symmetry [1]. In particular, La2-xAxCoIrO6 (A = Ca, Ba) shows exciting properties such as magnetodieletric effect [2] and cooperative octahedral breathing distortion [3]. However, the microscopic mechanisms governing its magnetic properties are not fully understood.

Through a detailed investigation of Co and Ir local electronic and magnetic structures in La1.5A0.5CoIrO6 (A = Ba, Ca) using X-ray absorption spectroscopy and X-ray magnetic circular dichroism we show that a competition between the different magnetic interactions underlies the stabilisation of magnetism in these compounds. A dominant antiferromagnetic coupling is responsible for the ferrimagnetic behaviour observed for the Ca-based sample below ~96 K, with the competing magnetic phases and the cationic disorder giving rise to a spin-glass state at low temperatures. On the other hand, the Ba-based compound has no evidence of long-range order down to its spin-glass transition temperature. The remarkably different magnetic properties observed for these compounds will be discussed in terms of the structural distortion that alters the strength of the Co-Ir couplings, with a relevant role played by the Co 3d eg-Ir 5d jeff=1/2 hybridisation.

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Flexure-induced strain control of antiferromagnetic domains in crystal membranes

Jack Harrison[1], Hariom Jani[1,2], Junxiong Hu[2], Sonu Hooda[2], Saurav Prakash[2], Zhiyang Zeng[1], Tim Butcher[3], Simone Finizio[3], Prof. Paolo Radaelli[1]
[1]University Of Oxford, Oxford, United Kingdom, [2]National University of Singapore, Singapore, [3]Paul Scherrer Institute, Switzerland

Magnetism 2, June 30, 2023, 09:30 - 10:30

Antiferromagnetic (AFM) materials are ideal candidates for spintronic devices due to their ultra-fast dynamics and relative immunity to external magnetic fields. The canted AFM α-Fe_2O_3 is a particularly promising system as it hosts a family of topological textures, namely (anti)merons and bimerons, at room temperature [1,2] and is predicted to host AFM skyrmions [3]. In addition, α-Fe_2O_3 exhibits long-range spin diffusion, a reasonably large spin-Hall magnetoresistance, and low Gilbert damping; crucial for low-energy ultra-fast magnetic dynamics [4-6]. Recently, we developed freestanding crystalline α-Fe_2O_3 membranes, which can be transferred to any desirable platform post-growth [7] and are inherently flexible, hosting large strains compared to attached thin films [8]. By creating a set of detached α-Fe_2O_3 membranes transferred onto Si_3N_4 substrates and imaging them using a scanning transmission X-ray microscope (STXM), we demonstrated that bends formed serendipitously during transfer lead to spatially-modulated magnetic states [7] (Fig a, b). Finite-element modelling of the bends link these magnetic variations to the flexure-induced membrane strain. Additionally, we utilised a strain cell to explore the effects of systematically applied uniaxial and biaxial strain on α-Fe_2O_3 membranes. We explored a wide temperature-strain phase space and demonstrated that strain can effectively tune the inherent spin-reorientation (Morin) transition and AFM domain orientations. This work is the first example of tuning the magnetic structures of freestanding AFM membranes via strain and demonstrates athermal nucleation of AFM topological textures, as well as further avenues of exploration that would utilise the flexibility of these systems, such as flexomagnetic effects or curvilinear magnetism.

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Stabilization of in-plane ferromagnetism at the surface of quantum critical Sr3Ru2O7

Dr Luke Rhodes[1], Mr Izidor Benedičič[1], Dr Masahiro Naritsuka[1,2], Dr Carolina Marques[1,3], Professor Peter Wahl[1]

[1]*University Of St Andrews, St Andrews, United Kingdom,* [2]*RIKEN Center for Emergent Matter Science, Saitama, Japan,* [3]*University of Zurich, Zurich, Switzerland*

Metals and Correlated Electron Systems 4, June 30, 2023, 15:00 - 17:00

Quantum critical systems are systems in which a phase transition occurs at zero temperature through quantum fluctuations that are driven by an external tuning parameter. These systems offer fascinating insight into correlated electron behaviour and often result in the stabilization of new emergent orders, such as unconventional superconductivity.

The paramagnetic metal $Sr_3Ru_2O_7$ shows evidence of quantum critical behaviour at magnetic fields close to 8 T, applied along the crystallographic c-axis, and is one of the cleanest systems in which this behaviour can be realized and experimentally studied. Close to the critical field, a new phase is stabilized in a narrow field region below 1 K [1]. Little is known about this phase except that it exhibits significant breaking of four-fold rotational symmetry when the field is tilted slightly away from the c-axis [2] and that the electronic anisotropy can be controlled by the in-plane component of the magnetic field [3].

Recent scanning tunnelling microscopy (STM) measurements studying the surface of $Sr_3Ru_2O_7$ [4,5] have observed that the surface already exhibits these properties; a breaking of the four-fold rotational symmetry that can be controlled via an external in-plane magnetic field, even at very small magnetic fields and at temperatures >10 K.

Here, I will discuss how these STM measurements provide strong evidence suggesting that the surface of $Sr_3Ru_2O_7$ hosts in-plane ferromagnetism, even without the application of an external magnetic field. Using a minimal tight-binding model that captures the electronic hopping, spin orientation, and spin-orbit coupling we simulate the continuum local density of states - a quantity that is directly comparable with STM measurements - and show that these simulations directly reproduce the qualitative evolution of the electronic states with field observed in STM. I will discuss the consequences and possible mechanisms for such a surface-induced magnetic order and potential implications for the quantum critical region of the bulk material.

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Structural and magnetic competition in (111)-oriented manganite superlattices

Fabrizio Cossu[1], Heung-Sik Kim[1], Igor di Marco[2], Julio do Nascimento[3], Vlado Lazarov[3]
[1]Kangwon National University - Department of Physics and Institute of Quantum Convergence and Technology, Chuncheon, South Korea, [2]Nicolaus Copernicus University - Department of Physics, Astronomy and Informatics, Toruń, Poland, [3]University of York - School of Physics, Engineering and Technology, York, United Kingdom

Helium and Complex Structured Materials, June 29, 2023, 11:00 - 13:00

Oxide heterostructures can host exotic phenomena and interesting phase competition in thin films and superlattices, because of symmetry breaking and quantum confinement. These phenomena include flat bands [1], magnetic anisotropy [2], exchange bias [3] and spin-glass [4,5]. Many of these phases are only latent in bulk, but emerge in ordered mixed-valent structures, such as superlattices. The (001)-oriented superlattice of two anti-ferromagnetic insulators LaMnO3 and SrMnO3 is a half-metallic ferromagnet with short periodicity, but an antiferromagnetic insulator with 2 or more unit cells [6,7,8]. Via ab-initio calculations, we predict that a (111)-oriented LaMnO3|SrMnO3 superlattice is a half-metallic ferromagnet in spite of its large thickness due to strain and charge transfer across the interface [9]. Magnetism dwells in the bulk-like regions rather than being a local interfacial effect. In particular, the maximum of the magnetisation is found inside the LaMnO3 region [9] (in (001)-oriented superlattices is at the interface [6,7,8]). As thickness grows, the coupling between Mn progressively shifts to antiferromagnetic in the Sr region, suggesting mixed magnetism, with possible applications for spintronics and magnetic sensing.
We compare also two space groups, which are found as the ground state of bulk LaMnO3 and bulk La2/3Sr1/3MnO3: Pnma and R3c, respectively. Their competition, tuned by in-plane strain and superlattice thickness, plays a role in the magnetic coupling and in the competition between orbital and charge order. This is due to the fact that Pnma naturally promotes A-type antiferromagnetism throughout the superlattice, which is linked to orbital order. Instead, the R-3c quenches the Jahn-Teller and supports breathing distortions, coupled to charge and spin oscillations, in a similar guise to interesting cases of Hund's metals and high-TC superconductors.

Magnetic coupling constants are obtained within the Heisenberg formalism via the magnetic force theorem, and show a large ferromagnetic coupling in the inner LaMnO3 region and a weakly antiferromagnetic coupling in the SrMnO3 region, see figure, suggesting mixed orders; finally, we estimate the Curie temperature via atomistic spin dynamics.

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Coherent Control of a Single Electronic Spin in a 2D Material at Room Temperature

Dr Hannah Stern[1], Dr Carmem Maia Gilardoni[1], Dr Qiushi Gu[1], Xiaoxi Deng[1], Simone Eizagirre Barker[1], Oliver Powell[1], Louis Follet[1], Professor Igor Aharonovich[2], Professor Mete Atature[1]
[1]University Of Cambridge, Cambridge, United Kingdom, [2]University of Technology Sydney, Sydney, Australia

Atomic, Molecular and Optical Physics, June 30, 2023, 09:30 - 10:30

Spin-active optical defects in solid-state materials are a leading material platform for quantum technology, such as quantum repeaters and sensors. A key requirement for successful application is access to coherent optical and spin transitions. Here, I present the quantum control at room temperature of a single spin qubit in a wide bandgap two-dimensional material, hexagonal boron nitride. Via optically detected magnetic resonance we determine a spin-triplet ground state. Using pulsed spin control, we demonstrate coherent spin oscillations for the spin qubit that last beyond 1 μs in the strong driving regime, indicating that the electronic spin state can be decoupled from the spin-rich nuclear environment, even at room temperature. These results open routes towards a room-temperature, two-dimensional spin-photon interface for quantum networks and sensing.

Efficient computation of optical properties of large-scale heterogeneous systems

Dr Joseph Prentice[1]
[1]*University Of Oxford, Oxford, United Kingdom*

1. Nonequilibrium Physics 2. Instruments and Applications, June 30, 2023, 15:00 - 17:00

The optical properties of large-scale (>1000 atoms) heterogeneous systems are of interest in several fields, from photovoltaics to biological systems. Computing such properties accurately from first principles, however, is challenging; even if only a small region is optically active, quantum mechanical environmental effects must often be included, and the cost of applying a quantitatively accurate level of theory is prohibitive. Here, I present recent work demonstrating how such calculations can be performed efficiently from first principles via two methods: an extension of the spectral warping method of Ge et al., and a novel combination of quantum embedding (specifically embedded mean-field theory) and linear-scaling (time-dependent) density functional theory. The accuracy and utility of these methods is demonstrated by applying them to systems including the molecular crystal ROY, chromophores in solution, and pentacene-doped p-terphenyl. The results pave the way for quantitatively accurate calculations to be performed on previously inaccessible large-scale systems.

Materials Optimisation for Next Generation Low Power Electronic Devices

Mr Ieuan Wilkes[1], Professor Keith McKenna[1]
[1]*University of York Physics Department, York, United Kingdom*

Magnetism 4, June 30, 2023, 15:00 - 17:00

In recent years, antiferromagnetic materials have become a more active area of research for their potential applications in memory devices [1]. These materials have an array of interesting spintronic properties, and can be used as a basis for (antiferromagnetic spintronic) memory storage devices [2]. These devices could offer unique advantages over existing computational architecture, including excellent energy efficiency compared to modern charge-based memory architecture, increased switching speeds and resistance to the influence of external stray magnetic fields [3], the latter of which MRAM devices struggle with [4]. In recent work we have investigated the use of density functional theory [5,6,7,8,9] for predictive modelling of the structure, magnetic order and magnetic anisotropy energy (MAE) of antiferromagnetic materials to guide selection and optimisation of materials for devices. Importantly for the calculation of MAE we include the contribution from the magnetic dipole energy [5]. Using this carefully validated approach we have also investigated the MAE of the noncollinear L12 Mn3Ir and D019 Mn3Ge antiferromagnets.

Directional Ballistics in Ultra-Pure Delafossite Metals

Michal Moravec[1,2], Graham Baker[2,3], Maja D. Bachmann[1,2], Philippa H. McGuinness[1,2], Markus König[2], Seunghyun Khim[2], Andrew P. Mackenzie[1,2]
[1]University of St Andrews, St Andrews, Scotland, [2]MPI CPfS, Dresden, Germany, [3]University of British Columbia, Vancouver, Canada

Metals and Correlated Electron Systems 2, June 29, 2023, 11:00 - 13:00

Studying electrical transport in extremely pure materials has lead to discovery of novel phenomena including the fractional quantum Hall effect or electron hydrodynamics. The delafossite metals, with their two-dimensional electronic structure and mean free paths in excess of 20 μm, are a recent addition to the ultra-pure materials class.

Here we study electrical transport in bars of varied width in delafossite metals PdCoO2 and PtCoO2. The bar-like structures are sculpted in two crystal orientations using the focused ion beam and sequentially narrowed across the width corresponding to the mean free path. We observe a cross-over from Ohmic to ballistic transport and gradual increase in resistivity anisotropy between the two orientations, as the channel is narrowed. This anisotropy is not allowed by the symmetry of the bulk crystal lattice; it is an example of symmetry lowering due to the impo- sition of shapes of finite size and the Fermi surface anisotropy [1]. We also complement our measurements with numerical solutions to the Boltzmann equation including the ARPES Fermi surface parametrisation. We obtain a good qualitative agreement with resistivity the data and estimate the strength of momentum-conserving scattering in the delafossite metals.

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Unconventional superconductivity underpinned by antiferromagnetism in $YbRh_2Si_2$

Lev Levitin[1], Jan Knapp[1], Marijn Lucas[1], Petra Knappova[1], Jan Nyeki[1], Brian Cowan[1], Andrew Casey[1], Kristin Kliemt[2], Cornelius Krellner[2], Manuel Brando[3], Christoph Geibel[3], John Saunders[1]
[1]Royal Holloway, University Of London, Egham, Surrey, United Kingdom, [2]Goethe University, Frankfurt am Main, Germany, [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Superconductivity 3, June 30, 2023, 15:00 - 17:00

We present the study of interplay between magnetism and superconductivity in a heavy-fermion metal $YbRh_2Si_2$, probed with high-resolution measurements of electrical impedance, ac susceptibility and heat capacity down to 0.2 mK, using ultra-sensitive SQUID-based experimental techniques.

In addition to the well-established antiferromagnetism (AFM) below the Néel temperature T_N = 70 mK [1] with small staggered moments μ_e ~ 0.002μ_B [2], we observe a second AFM order with onset T_A = 1.5 mK, stabilised by the hyperfine interactions in ^{171}Yb and ^{173}Yb and exhibiting much larger moments μ_e ~ 0.1μ_B [3]. From signatures in calorimetry and magnetoresistance we map the suppression of T_N (down to 4 mK at 50 mT) and T_A (down to 0.5 mK at 30 mT) with magnetic field applied in the ab plane of the tetragonal $YbRh_2Si_2$ single crystals.

The superconductivity manifests below 10 mK as zero resistance or a partial resistance drop. Simultaneously the imaginary component of the sample impedance develops, that we attribute to the kinetic inductance. The frequency dependence of the complex impedance, the absence of signatures of superconductivity in the heat capacity between 2 and 10 mK [3] and the small shielding volume [4] point towards inhomogeneous superconductivity. Different transport signatures of superconductivity exhibit distinct dependence on the magnetic field, both Pauli-limited and beyond the Pauli limit, suggestive of spin-triplet pairing and multiple superconducting order parameters, possibly with non-trivial topology.

Importantly the superconductivity is switched off at the critical field of the primary AFM order; moreover the impedance abruptly changes across the T_A(H) phase boundary between the two magnetic phases. We conclude that the superconducting order parameters that form in $YbRh_2Si_2$, are sensitive to the magnetic state of the sample and require the presence of AFM order. An intriguing scenario is spin-triplet pairing mediated by ferromagnetic fluctuations.

It is natural for the superconductivity with very low critical temperature to be sensitive to inhomogeneities, such as strain and magnetic domain structure. Controlling these opens the door to stabilising homogeneous versions of the many superconducting states revealed in our experiments, with prospective applications to topological superconducting quantum devices.

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The quantum muon as a probe of magnetic frustration

Stephen Blundell[1]
[1]*University Of Oxford, Oxford, United Kingdom*

Magnetism 1, June 29, 2023, 09:30 - 10:30

The unitary evolution of a quantum system preserves its coherence, but interactions between the system and its environment result in decoherence, a process in which the quantum information stored in the system becomes degraded. A spin-polarized positively charged muon implanted in a fluoride crystal realizes such a coherent quantum system, and the entanglement of muon and nearest-neighbor fluorine nuclear spins gives rise to an oscillatory time dependence of the muon polarization that can be detected and measured. The decohering effect of more distant nuclear spins can be modelled quantitatively, allowing a very detailed description of the decoherence processes coupling the muon-fluorine “system” with its “environment,” and allowing us to track the system entropy as the quantum information degrades. This approach can be used to think about how the quantum muon couples to the magnetic degrees of freedom in a spin liquid.

Characterization of Titanium-Nitride Thin Films & Design of Kinetic Inductance Travelling Wave Parametric Amplifier

Searbhán Ó Peatáin[1], Dr Joshoua Esmenda[1], Dr Chung-Ting Ke[3], Dr Jonathan M Williams[2], Dr Sergey Kafanov[1], Prof ChiiDong Chen[3], Prof Yuri A Pashkin[1]
[1]Lancaster University, United Kingdom, [2]NPL, Teddington, United Kingdom, [3]Academia Sinica, Taipei, Taiwan

Superconductivity 2, June 29, 2023, 11:00 - 13:00

Thin superconducting films demonstrate a non-linear inductance due to the inertia of charge carriers. This `kinetic inductance' can be used for the creation of travelling wave parametric amplifiers (TWPA's) formed solely of a superconducting transmission line. These devices have their non-linear inductance modulated by a strong pump tone while power flows to a weaker signal tone by some wave-mixing interactions. It has been shown that thin films approaching the superconductor-insulator-transition show anomalously high kinetic inductance, perfect for this type of application. We discuss here characterization of Titanium Nitride (TiN) films, and from this the design of kinetic inductance TWPA devices.

The 2D Ferromagnetic Extension of a Topological Insulator

Mr. Philipp Kagerer[1], Dr. Celso I. Fornari[1], Mr. Sebastian Buchberger[1,2], Mr. Begmuhammet Geldiyev[1], Prof. Hendrik Bentmann[1,3], Prof. Friedrich Reinert[1]
[1]JMU Wuerzburg, Physikalisches Institut (EP7), Wuerzburg, Germany, [2]University of St. Andrews, UK, St. Andrews, United Kingdom, [3]Center for Quantum Spintronics, NTNU Trondheim, Trondheim, Norway

Topological Materials 1, June 29, 2023, 11:00 - 13:00

3D topological insulators (TI) are known to have a topological non-trivial band structure protected by time reversal symmetry, which also guarantees the metallicity of the surface. Consequently, it is sufficient to break this symmetry only locally at the surface of the sample to gap out the topological surface state (TSS), leading to a variety of novel topological effects, e.g. an axion term in the electromagnetic response and quantized spin-selective edge channels.

While most experimental approaches to date have aimed to introduce magnetism globally, we present the first experimental realisation of the ferromagnetic extension (1), a design directly interfacing a 3D TI with a two-dimensional non-trivial magnet. Utilizing a single septuple layer MnBi2Te4 on the prototypical TI Bi2Te3, we establish a stable 2D ferromagnetic ground state and introduce a sizeable magnetic exchange gap in the TSS (2). By means of photoemission spectroscopy and X-ray absorption spectroscopy, we will demonstrate the congruence of gap closing and magnetic order parameter and present means of manipulating the magnetism in the surface layer by further engineering of the MBE growth process.

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Chemically controllable magnetic transition temperature and magneto-caloric properties in MnZnSb based compounds

Jonathan Alaria[1]
[1]*University of Liverpool, Department of Physics & Stephenson Institute for Renewable Energy, Liverpool, United Kingdom*

1. Nonequilibrium Physics 2. Instruments and Applications, June 30, 2023, 15:00 - 17:00

A viable compound for magnetic refrigeration at ambient temperature must present a large change in magnetic entropy, with minimum hysteresis and should be composed of earth abundant and non-toxic elements. [1] Recently a computational proxy was developed to identify new magnetocaloric materials whereby first principle structure relaxation is carried out with and without spin polarization to ascertain the degree of magnetic deformation. [2]

By applying this method to ferromagnets in the PbFCl family we found magnetic deformation of around 2% which is similar to other magnetocaloric compounds. We therefore have focussed our experimental study on MnZnSb, which is reported to be an itinerant ferromagnet with a second order phase transition and Curie temperature about room temperature. [3] Detailed magnetization measurements were carried out and Arrott analysis (Fig 1. a)) yields a Curie temperature of 304K, with the system being described as one universality class across all order parameters and identified as '2-dimensional long-range.' We find a reasonably large magnetic entropy change of 4.5 Jkg-1K-1 with a relative cooling power of 153 Jkg-1; which is comparable to second order compounds with about room temperature transition temperatures.

Temperature dependant powder neutron diffraction was used to investigate the origin of the significant magnetic entropy change around the magnetic transition which is attributed to the release of crystallographic strain through the magnetic transition. We identify the c/a parameter as an accurate crystallographic proxy to control the magnetic transition (Fig. 1 b)). Using this concept, chemical substitution on the square-net allows to experimentally tune the Curie temperature over a broad temperature span between 252-322 K (Fig. 1 c)). A predictive machine learning model for the c/a parameter is developed to guide future exploratory synthesis.

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Current quantization due to the a.c. coherent quantum phase slip effect

Rais Shaikhaidarov[1]
[1]*RHUL, Egham, United Kingdom*

Superconductivity 2, June 29, 2023, 11:00 - 13:00

The AC Josephson effect was observed experimentally in 1963 Ref. [1] as quantized voltage steps from photon assisted tunnelling of Cooper pairs. Shapiro steps appear at voltages Vn=Φ0fn, where f is the microwave frequency, Φ0 is the flux quantum and n is an integer. The physically dual effect, the AC coherent quantum phase slip (CQPS), photon assisted tunnelling of magnetic fluxes through a superconducting nanowire, was predicted to show itself as quantized current steps. The steps form at current values In=Q0f n, where the charge quantum Q0=2e is the charge of a Cooper pair. We report the direct observation of the dual Shapiro steps in a superconducting NbN nanowire under microwave drive. The FIB image of sample is shown on Fig.1a. A typical I-V curve measured at a base temperature of 10mK demonstrates distinct superconducting behavior. Under microwave excitation I-V curve is drastically modified, current steps develop. Fig.1b,c shows steps in the measured I-V characteristic at frequency f = 14.924 GHz.

Figure 1: a) The superconducting 100 nm wide wire with a constriction of 20x50nm2 is embedded into the circuit with compact NbN inductances and Pd resistances. The circuit is connected to current, I+/I-, and voltage V+/V- leads. b) and c) Quantized current steps. Horizontal lines show the expected position of plateaus at $nQ0f$ where Q=2e Cooper pair charge and f=14.924GHz. Microwave power corresponds to AC current Iac 7nA and 14nA for b) and c) correspondingly.

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Topological magnons driven by the Dzyaloshinskii-Moriya interaction in the centrosymmetric ferromagnet Mn5Ge3

Dr. Manuel Dos Santos Dias[1]
[1]*STFC Daresbury Laboratory, Warrington, United Kingdom*

Magnetism 1, June 29, 2023, 09:30 - 10:30

The phase of the quantum-mechanical wave function can encode a topological structure with wide-ranging physical consequences, such as anomalous transport effects and the existence of edge states robust against perturbations. While this has been exhaustively demonstrated for electrons, properties associated with the elementary quasiparticles in magnetic materials are still underexplored. Here, we show theoretically and via inelastic neutron scattering experiments that the bulk ferromagnet Mn5Ge3 hosts gapped topological Dirac magnons. Although inversion symmetry prohibits a net Dzyaloshinskii-Moriya interaction in the unit cell, it is locally allowed and is responsible for the gap opening in the magnon spectrum. This gap is predicted and experimentally verified to close by rotating the magnetization away from the c-axis. Hence, Mn5Ge3 is the first realization of a gapped Dirac magnon material in three dimensions. Its tunability by chemical doping or by thin film nanostructuring defines an exciting new platform to explore and design topological magnons.

Integration of semiconductor Josephson junctions in superconducting quantum circuits

Dr Malcolm Connolly[1]
[1]*Imperial College London, London, United Kingdom*

Topological Materials 1, June 29, 2023, 11:00 - 13:00

Nanostructured low-dimensional materials provide an exciting sandpit for exploring fundamental ideas in condensed matter physics and could potentially enable next-generation quantum devices. Superconducting quantum circuits with integrated mesoscopic semiconductor Josephson junctions (JJs) have emerged as a versatile platform for realising hybrid qubits with gate-tuneable properties and for studying interactions between quasiparticle excitations and microwave light. In this talk I summarise progress towards realising these experiments with scalable quantum circuits hosting V-VI topological insulators and III-V 2D electron gases [1,2]. I will discuss some of the main challenges with using strong spin-orbit interactions in these materials to realise highly-coveted topological phases in the presence of disorder and strong global magnetic fields, and describe some possible routes forward using magnetic materials [3].

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Antimony trisulfide: from local structural transitions to programmable photonics

Assoc Prof Robert Edward Simpson[1], Ms Ting Yu Teo, Dr Li Lu, Dr Yunzheng Wang, Dr Jing Ning, Dr Parikshit Moitra, Dr Ramon J. Paniagua Dominguez, Dr Zhao Gang Dong, Dr Arseniy Kuznetsov, Assoc Prof Joel Yang
[1]*University Of Birmingham, Birmingham, United Kingdom*

Surfaces, Interfaces and Thin Films, June 30, 2023, 11:00 - 13:00

Thin films that exhibit substantial property contrast between different structural phases are of interest for data storage and programmable photonics applications. The most successful data storage materials, such as those that lie along the GeTe-Sb2Te3 pseudo-binary compositional tie-line, have a small bandgap and concomitantly, a large optical absorption in the near infrared and visible spectrum. New phase change materials with a wider bandgap need to be developed for visible and N-IR photonics applications. Antimony trisulfide (Sb2S3) is an Earth abundant material that is transparent to visible and near infrared light (N-IR). Switching the material between amorphous and crystalline states causes radical property changes that deem it useful for programming the response of visible and N-IR photonics devices. We have demonstrated how Sb2S3 can be used to program high resolution micro-displays, dielectric metasurfaces, hyperbolic metamaterials, waveguides, and all-optical neural networks.

Most typical phase change data storage materials usually have just two stable structural states at room temperature. Thus, the intrinsic optical constants can be switched between two states. In contrast, the optical constants of Sb2S3 can be continuously tuned across a wide range of values by using successively higher laser pulse energies to switch the material. We show using density functional theory molecular dynamics (DFT/MD) simulations that this continuous tuning is likely due to a bond hierarchy in the Sb2S3 crystal. The coordination of Sb atoms is continuously tunable when it is melted at successively higher temperatures. In the crystalline state, Sb is close to 6-fold coordinated by S, but when heated well-above the melting point and quenched rapidly, the coordination can change to 3-fold. The average Sb coordination can be continuously tuned from six-fold to three-fold using temperature.

The first part of this presentation will discuss the properties of Sb2S3 and show how they can be exploited for programming photonics devices. The second part of the presentation will examine the Sb2S3 crystal and discuss the tuneability of the Sb2S3 optical properties.

Topological properties of a one-dimensional excitonic model combining local excitation and charge transfer

Dr. Jianhua Zhu[1,2], **Dr Wei Wu[2]**
[1]School of Physics, Peking University, Chengfu Road 209, Haidian, Beijing 100871, China, [2]UCL Department of Physics and Astronomy, University College London, London, United Kingdom

Topological Materials 2, June 30, 2023, 11:00 - 13:00

Excitons (electron-hole pairs) not only play a vital role in physics but also for many important applications in Bose-Einstein condensation, photonics, carbon-nanotubes, two-dimensional materials, solar cells and light-emitting diodes (LED), which need to be understood properly from a microscopic perspective [1]. One-dimensional chain structures consisting of atoms, molecules, quantum dots, dopants have recently attracted much attention due to their interesting topological properties [2]. The combination of the two, excitons in one dimension, is of great interest for fundamental studies of low-dimensional optics and photonics from a bosonic point of view [3].

Our previous work based on a combination of time-dependent density-functional-theory (TDDFT) calculations and tight-binding model has shown a significant improvement compared with the TDDFT calculations for molecular dimers. Here we have computed the Zak phase to characterize the topological properties in this one-dimensional excitonic model [3], which takes into account dimerisation, local and charge-transfer excited states. We have mapped our previous model [3] to a more straightforward presentation as shown in Fig.1. There are four hopping parameters (t_1,t_2,t_1',t_2'), which can be varied to give rise to a rich spectrum of physics. By turning on more than one parameter, we can find (i) the topological phase could exist even for a uniform chain, (ii) topologically nontrivial flat bands can arise, suggesting an interesting correlation between flat bands and topology, (iii) exotic fractional phases, which might be due to the quantum interference between chiral states, and (iv) an interesting phase transition due to second-order hopping. Our calculations show interesting topological phase transition when tuning the hopping parameters. As shown in Fig.1, we can see there is an interesting phase transition at $|t_1t_2|=|t_1't_2'|$, which indicates a second-order hopping event between the neighboring local excited states (LE1 and LE2). We have also developed the concept of effective chiral states (a linear combination of individual excitonic states) to interpret our calculations. Our model is sufficiently general to take into account both LE and CT excitations, which would exist universally in one-dimensional chain structures formed by physical unit such as atom, molecule, dopant, and quantum dot.

Figure 1: (a) coupling map. (b) the Zak phases as function of t_1 and t_2, in which there is a phase transition at $|t_1t_2| = 1$.

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Effects of cavity and atomic decay rates on efficiencies of quantum memory

Takla Nateeboon[1], Chanaprom Cholsuk[2], Tobias Vogl[2,3], Sujin Suwanna[1]
[1]Department of Physics, Faculty of Science, Mahidol University, Bangkok, Thailand, [2]Abbe Center of Photonics, Institute of Applied Physics, Friedrich Schiller University Jena, Jena, Germany, [3]Fraunhofer-Institute for Applied Optics and Precision Engineering IOF, Jena, Germany

Atomic, Molecular and Optical Physics, June 30, 2023, 09:30 - 10:30

Quantum memories are essential for the storage and synchronization of photonic qubits travelling in a long-distance quantum network of quantum repeaters. When a quantum memory maps the state of light to that of matter for storage, the process is subject to decay and losses, such as the decay of population matter qubits in electronic states and the decay of photonic states in a cavity where the quantum memory is hosted. Three types of efficiency in quantum memory are investigated: the writing efficiency from a photonic state to a matter qubit, the reading efficiency back from the matter qubit to the photonic state, and the global efficiency of the entire process, including effects during storage. Here, we investigated how cavity and atomic decay rates affect the efficiency of adiabatic-type quantum memory from a single lambda-type atom. We found that the decay rates of cavity field and coherence limit writing and reading efficiencies, while the atomic population decay rate limits global efficiency. We calculated the situations where quantum memories created from titanium bi-vacancy and molybdenum bi-vacancy defects in hexagonal boron nitride could operate at a perfect writing efficiency. We found that the cavity's quality factor used to host these defects has to be in the order of 10^5 for the memory to reach the ideal efficiency. These results will help future experiments in pursuit of realizing quantum memory.

Modelling strain experiments in unconventional superconductors

James Annett[1], Macauley Curtis[1], Martin Gradhand[1,2]
[1]*University Of Bristol, Bristol, United Kingdom,* [2] *Johannes Gutenberg University Mainz, Germany*

Superconductivity 3, June 30, 2023, 15:00 - 17:00

Strain experiments can provide a unique experimental probe of pairing symmetry in unconventional superconductors. For example, recent (100) uniaxial strain experiments in Sr2RuO4 show a dramatic increase in Tc from 1.5 to 3.2K, and also suggest that the temperatures of time reversal symmetry breaking TRSB transition and the superconducting Tc become different in strained samples[1]. Using a simple one-band model of the band structure of Sr2RuO4 near to the van Hove singularity at the strain induced topological Fermi surface transition we find that a d+ig pairing symmetry provides the best overall agreement to the (100) uniaxial strain experiments[2]. Extending this model to the cases of c-axis compression and a-b plane shear strain allows further comparisons to a wider set of experiments on Sr2RuO4[3. Similar predictions for strain experiments other unconventional superconductors are also made within this same model.

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Poster presentations

Exploring topological excitations of S=1/2 kagome ferromagnets using inelastic neutron scattering

Miss Amie Troath[1]

[1]*University of Birmingham, United Kingdom*

S= ½ kagome ferromagnets have been theoretically predicted to exhibit interesting physical properties such as the quantum Hall effect.1 Inelastic neutron scattering (INS) allows us to observe the band structure of the magnetic excitations, which are related to the properties of such materials.2 Material synthesis remains a challenge, given that purely inorganic systems are subject to atomic site disorder.3 In the last decade, the literature has shown the experimental synthesis of a S= ½ kagome ferromagnet with a metal-organic framework (MOF) as a means to avoid this unfavourable atomic site disorder.2 MOF systems consist of inorganic layers separated by organic linkers as a means to realise a quasi-two-dimensional magnetic model. In this poster I shall present two S= ½ kagome ferromagnets with a P3 spacegroup, MOF-bpy3 and MOF-bipy4. Both systems consist of Cu2+ ions which reside on the corners of the breathing kagome structure, with carbonate ions within these triangles to facilitate the superexchange interactions between Cu2+ ions. There exists also perchlorate ions within the hexagonal channels of the kagome network, acting as counter anions. We have two in-plane ferromagnetic superexchange interactions as a result of this breathing kagome network. MOF-bpy has an additional interaction between the kagome planes of a weak antiferromagnetic nature, whereas the linker in MOF-bipy does not allow for this third interaction and stacking of inorganic-organic layers is achieved through π-π interactions.

INS measurements of MOf-bpy on LET are dominated by phonon scattering and so I will demonstrate how SpinW can be used to simulate the powder INS spectrum to direct the design of future INS experiments.5 I will also present how this software can be used to determine how robust the features of the powder INS simulation are to the variation of the magnitude and nature of the exchange interactions.

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Probing the Magnetization Distribution in Ferrite Nanoparticles with Magnetic SANS

Dr Dirk Honecker[1]
[1]*ISIS Neutron and Muon Source, STFC, Didcot, United Kingdom*

Tailoring magnetic nanoparticles (MNPs) by choosing a suitable combination of size, shape, and material is the basis in realizing various technological, biomedical, or environmental applications.
For optimal performance, it is crucial to interrelate their macroscopic characteristics with the structural and magnetic properties of MNPs. For example, disorder effects crucially determine the magnetic heating performance of MNPs for hyperthermia, magnetic particle imaging, and catalysis applications [1].
This contribution presents the advantages of small-angle neutron scattering for investigating the nanoscale distribution of spin disorder in the relevant mesoscopic size range from 1 to a few hundred nanometres [2]. In conjunction with complementary methods, a detailed multiscale characterization of the chemical morphology and magnetization distribution in MNPs is available. In particular, the analysis reveals the internal magnetization profile of the nanoparticles and the field-dependent magnetization process near the structurally defective surface of MNPs [3]. Such intriguing details are missing in the classical model, which considers MNPs as a static two-phase system with a collinear magnetized core and a structurally disordered and magnetically dead surface.
Finally, we give our perspective on how future small-angle scattering experiments in combination with micromagnetic simulations could help to obtain further insight in the performance of MNPs [4].

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THE O(N) LOOP MODEL ON QUASICRYSTALS

Ms. Shobhna Singh[1], Jerome Lloyd[2], Dr. Felix Flicker[1]
[1]School of Physics and Astronomy, Cardiff University, United Kingdom, [2]Department of Theoretical Physics, University of Geneva, Geneva, Switzerland

In statistical physics, universality is the observation that there are properties for a large class of systems that are independent of the details of the system at a critical point. A universality class is a collection of mathematical models which may differ dramatically at finite scales, but their behavior will become increasingly similar as the continuum limit is approached. In particular, asymptotic phenomena such as critical exponents will be the same for all models in a class.

In this work I will consider how universality survives in an aperiodic setting: the Ammann-Beenker tiling which has quasicrystalline symmetries. These have the symmetries of certain quasicrystals (created in V-Ni-Si alloys), optical lattices, and twisted trilayer graphene. Considering the O(n) loop model on the AB tiling, I consider in detail two special limits - the Hamiltonian cycle and the fully packed loop (FPL) model. I compare the critical behavior of the latter with its equivalent in the periodic square lattice.

The main use of the result is that our construction suggests a method of translating classical statistical models such as fully packed loops, O(n) spin models, and quantum models like quantum dimer model from their well-studied periodic settings to this new aperiodic setting. It provides an important test of a basic assumption of condensed matter physics -- that large scale phenomena should be independent of the underlying lattice structure.
Further there is a possibility to study the approach to criticality from a new direction and to study a variety of strongly correlated problems which were previously intractable on quasicrystals. These include cases of physical relevance in real materials, such as magnetism and strongly correlated electronic phenomena.

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Signatures of Orbital Selective Mott state in doped Sr3Ru2O7

Buddhadeb Debnath[1], Shantanu Mukherjee[1]
[1]*IIT Madras, Chennai, India*

Bilayer Strontium Ruthenate Sr3Ru2O7 is a strongly correlated electronic system that shows diverse electronic and structural phases. Upon doping with Mn, an orbital selective Mott phase is observed before the material transitions to a Mott insulating state. Additionally, Mn doping leads to the emergence of an anti ferromagnetic (AFM) state with q_{AFM} =(pi/2,pi/2) ordering wavevector. Quasiparticle interference (QPI) experiments find a sharp but highly dispersive peak at the AFM wavevector. Another set of QPI peaks is observed at q^{*}=(pi,0) possibly due to a charge order effect. In this work we utilize a tight binding model relevant to Mn doped Sr3Ru2O7, and show that the origin of observed orbital selective Mott phase is inherently dependent upon the presence of a strong onsite exchange interaction and oxygen octahedral rotation suppression induced by the Mn doping. We further find that the experimentally observed QPI spectra including the peaks at q_{AFM}, and q^{*} wavevectors can be concomitantly explained within this formalism.

Soft X-ray angle-resolved photoelectron spectroscopy with a momentum microscope at Diamond Light Source

Dr Deepnarayan Biswas[1], Dr Matthias Schmitt[2], Dr Olena Tkach[3], Prof Ralph Claessen[2], Prof Gerd Schönhense[3], Dr Tien-Lin Lee[1]

[1]Diamond Light Source Ltd., Didcot, United Kingdom, [2]University of Würzburg, Germany, [3]University of Mainz, Germany

Angle-resolved photoelectron spectroscopy (ARPES) has become a mainstream technique for determining band structures of crystalline materials. The majority of the ARPES experiments are performed with excitation energies below ~120 eV to harness the higher photoionisation cross-sections and better energy and (in-plane) momentum resolutions. These advantages come, however, at a price that the very short electron mean free paths severely limit the bulk sensitivity and lead to ill-defined out-of-plane electron momentum (kz). It is therefore desirable to extend ARPES to the soft X-ray (SX) range, which opens up the opportunity for probing unconventional electronic structures at buried interfaces [1]. Moreover, the improved kz resolution makes ARPES more suitable for studying 3D electronic systems, as best exemplified by Weyl semimetals [2].

We are currently commissioning a SX-ARPES end-station at Beamline I09 [3] at Diamond Light Source. It is equipped with a state-of-the-art momentum microscope (MM). Unlike conventional hemispherical analysers, MMs preserve the momentum view and resolution irrespective of the excitation energy [4], which is particularly advantageous to ARPES performed at high energies. In addition, MMs enable selective studies of micron/sub-micron sized sample areas using field apertures. Furthermore, our MM is uniquely designed to use a single hemispherical analyser followed by a time-of-flight section fitted with a fast delay-line detector as a combined energy filter [5], resulting in highly efficient data collection. In this poster, we will present the end-station design, preliminary results from the commissioning of the MM, and the potential applications of this new facility to quantum materials research.

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Homogeneous, Isotropic, Three-body Backflow Correlation in Quantum Monte Carlo Simulations.

Clio Johnson[1]
[1]*Lancaster University, Lancaster, United Kingdom*

In the field of quantum Monte Carlo simulations (QMC), which uses random sampling methods to solve the many-body Schroedinger equation, there are two methods often used in tandem: Variational Monte Carlo (VMC), and Diffusion Monte Carlo (DMC). VMC iteratively updates a configuration of electron positions and optimises other free parameters in a trial wavefunction to produce optimised wavefunctions and variational ground state energies. DMC propagates a set of walkers stochastically through imaginary time, their density is used to recover an approximation to the ground state wavefunction. Since their density is positive, walkers are constrained from moving across the nodal surfaces of the wavefunction, leaving the nodes fixed and in approximate positions. This motivates research into techniques for first optimising the nodal surface of a wavefunction using VMC before using DMC to produce results. One well used technique for doing this is backflow, first developed for studying Helium, backflow involves displacing particle positions within a Slater determinant by an amount dependent on the entire configuration of particles. Typically, in VMC, the nodal surface is solely determined by a single Slater determinant, in a Slater-Jastrow wavefunction. Results obtained by Holtzmann and Moroni suggest that recursively performing two-body backflow displacements can improve ground state energies in QMC. However, this recursive technique proves computationally expensive. This may be mitigated by implementing higher order backflow terms to achieve the same effect. This project is implementing a three-body backflow displacement for use in studying 2D Fermi gases, alongside existing two-body and particle-Ion displacements.

High Resolution Imaging of Silicon Vacancy Colour Centres in Diamond Using 4D-STEM and Electron Ptychography

Mr Aidan Horne[1], Mr Xiaopeng Wu, Dr Ben Green, Dr Peng Wang
[1]*University of Warwick, Coventry, United Kingdom*

SiV colour centres appear in diamond as an interstitial site between two vacant carbon sites and have gained a lot of interest recently due to their potential uses in quantum computing. This potential comes from its capabilities as a coherent single photon emitter. In order to effectively implement these in colour centres, it is important that their nature is understood in terms of position within lattice as well as chemical behaviour all at a high resolution.

In this research, electron ptychography is used to image silicon vacancy (SiV) colour centres at a high atomic resolution in order to understand its atomic lattice and chemical behaviour. Electron ptychography, since being launched to a state of popularity within the microscopy community due to advances in superfast pixelated detectors has consistently demonstrated its capabilities at many tasks. From cryogenic biological samples and low dose imaging to ultrahigh resolution imaging and high Z contrast imaging. These last two are what makes the technique so useful for this research, since the most important factors to consider here is the ability to differentiate between the silicon and carbon lattice sites at a high resolution in order to locate where the silicon lattice sites sit within the diamond lattice. The sample preparation was done using bulk implantation into single crystal diamond followed by high temperature annealing. The TEM lamella samples were prepared using a Tescan FIBSEM. 4D-STEM experiments will be performed on a double aberration-corrected ARM200F STEM with an ultrafast Medipix detector.

Novel electronic structures from near-surface stacking faults

Dr Matthew Watson[1], Mr Mihir Date[1,2], Dr Alex Louat[1], Dr Cephise Cacho[1], Dr Niels Schröter[2]
[1]*Diamond Light Source, Didcot, United Kingdom,* [2]*Max Planck Institute of Microstructure Physics, Haale, Germany*

Angle-resolved photoemission spectroscopy (ARPES) measurements of transition metal dichalcogenides typically reveal both sharp features from the quasi-2D bands, and much broader spectral weight from the 3D bands, due to the intrinsic kz -uncertainty in photoemission. Here we show that in several well-known “2H" transition metal dichalcogenides, some regions of the cleaved sample surfaces show - unexpectedly and anomalously - a finite number of sharp dispersions, instead of the expected broad 3D states. The quantisation of these states, which we have found in “2H"-NbS_2, TaS_2 and MoS_2, is reminiscent of layer-quantisation effects seen in thin films or flakes, and their 2D nature is confirmed by photon energy dependent measurements. The spectra can vary dramatically in different positions on the sample, on the length scale of several microns, and we find different numbers of quantised features even within a single sample cleave. We speculate that these novel electronic structures derive from near-surface stacking faults, breaking the periodicity along the c axis near the surface. The results emphasise the new insight from doing micro-ARPES even on well-known materials.

Fullerene Thin Films as a Route to Skyrmion Nucleation

Mr Colin Kirkbride[1], Ms Sara Villa[1], Dr Kayla Fallon[1], Mr Christopher Barker[2], Prof Christopher Marrows[2], Prof Stephen McVitie[1]
[1]*University Of Glasgow, Glasgow, United Kingdom,* [2]*University of Leeds, Leeds, United Kingdom*

Driving the development of novel magnetic data storage is the need for low energy, high density materials with stable and reliable read, write and storage states. A potential solution lies in the domain of skyrmion-based racetrack memories which demands the reliable and controlled nucleation of skyrmion spin states [1] . This can be achieved using current injector devices, yet a major issue lies in post-nucleation depinning of single skyrmions from the injector device without forcing larger domain expansion [2]. Instead, an alternative approach is to spatially manipulate the strength of magnetic anisotropy and the Dzyaloshinskii-Moriya interaction. This has been shown using artificial defects [3], however an approach based on fullerene spinterfaces could provide an alternative non-destructive deposition-based solution through induced molecular anisotropy enhancement [4].

In this work, we characterise the effect of fullerene thin films on the formation of domains in the ferromagnetic multilayer system Ta(25Å)/[Pt(7Å)/A/Ir(7Å)]5/B where A is a magnetic CoB film with either 12Å or 14Å; and B is a capping layer of either C60(150Å)/Al(50Å) or Pt(20Å). Using a range of Lorentz transmission electron microscopy techniques, we measure the magnetic domain wall structure and show a reduction in periodicity induced by the fullerene film as in Fig 1. We relate this to a change in the effective anisotropy and support this with SQUID-VSM and MFM measurements. Overall, this work motivates further study of fullerene films on synthetic antiferromagnetic systems which have already shown significant skyrmion formation potential.

Molecular dynamics study on the relation between atomic structure and temperature of Mg-Zn alloys for metal air batteries electrodes

Mr. Hemant Kumar Limbu, Dr. Gavin Mountjoy
[1]*University Of Kent, Canterbury, United Kingdom*

Mg-Zn alloys which is a potential candidate for metal-air batteries electrodes have been studied using Classical Molecular dynamics modelling. The investigation at different temperatures using GULP, and DLPOLY software showed that the density of intermetallic compounds Mg51Zn20, Mg21Zn25, Mg4Zn7, MgZn2, and Mg2Zn11 vary with temperature. The intermetallic compounds change its atomic structure with change in temperature.

Superconductivity at 90 K in a lanthanum hydride film synthesised using elemental lanthanum and ammonia borane at 95 GPa

Mr Sam Cross[1]
[1]*University of Bristol, Bristol, United Kingdom*

The discovery of superconductivity in sulfur hydride in 2015 with Tc = 203 K at 155 GPa reignited the search for high temperature superconductivity in high pressure hydrides [1]. Record Tc was later reported in lanthanum hydride, LaH10, with Tc = 250 K at 180 GPa [2,3]. Synthesis of hydrides at these pressures is challenging, achieved by laser heating a precursor with a hydrogen donor in a diamond anvil cell (DAC). However, often multiple superconducting hydride phases coexist, leading to a cascade of transitions in resistivity measurements. Coupled with inhomogeneous conditions on laser heating, the isolation of clean, ideally single-phase, samples highlights a major challenge in order to reliably study the superconducting properties. A recent XRD study of lanthanum hydride phases has identified only two phases at ~100 GPa, LaH3 and La4H23, with significant phase mixing observed at higher pressures e.g LaH4, LaH6, LaH9, LaH10 in the range 140 – 176 GPa [4]. In this work I present the formation of a clean lanthanum hydride with a single transition at ~ 90 K, by laser heating a lanthanum film with ammonia borane at 95 GPa. Superconductivity is evidenced in zero-field and field dependent resistance measurements. I will outline the synthesis procedure and high-pressure transport techniques, and discuss the possible nature of the observed superconductivity.

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Exploration of novel quantum phases and large magnetic anisotropy energy in low-spin d5 perovskites: Bulk and Ultra-thin films

Mr Amit Chauhan[1], Mr Birabar Ranjit Kumar Nanda
[1]*Indian Institute Of Technology Madras, Chennai, India* [2]*Indian Institute Of Technology Madras, Chennai, India*

The crystalline solids are often a playground to generate novel quantum states which hold the key for next generation technological applications in the area of electronics, quantum information and quantum computation. In this talk we shall investigate the electronic structure of iridates and other low-spin isovalent members. The competition between onsite Coulomb repulsion (U) and spin-orbit coupling (SOC) leads to exotic quantum phases in the 4d and 5d transition metal oxides. By formulating a realistic multi-orbital Hubbard model and performing SOC tunable DFT+U calculations on the bulk and ultra-thin films of prototype system SrIrO3, we present eight electronic and magnetic phases in the U-SOC space for the family of low-spin bulk d5 perovskites. With reduced dimensionality we observe six unique phases. In the weak correlation regime, the film terminated by IrO2 layers exhibits multiple Dirac states. Furthermore, in the strong correlation regime, we estimate large and in-plane magnetic anisotropy energy (MAE) and qualitatively explain its underlying origin by carrying out a second-order perturbative analysis of SOC. The existence of large MAE in the ultra-thin films makes them promising candidates for magnetic memory and storage devices.

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Theoretical investigation on topologically robust edge-states in a harmonic synthetic dimension and its experimental realisation.

David Reid[1], Mr Chris Oliver[1], Dr Aaron Smith[1], Mr Tom Easton[1], Dr Grazia Salerno[2], Prof Nathan Goldman[3], Dr Giovanni Barontini[1], Dr Hannah Price[1]

[1]University Of Birmingham, Birmingham, United Kingdom [2]Aalto University, Espoo, Finland [3]Universite Libre de Bruxelles, Brussels, Belgium

There has been significant interest in topological physics since the discovery of the quantum Hall effect. The robustness of topologically protected phenomena, including the quantum Hall effect, naturally tailors it to future application. Notably applications have been found in metrology, where the SI units have been re-defined using the effect [1]. There has been a plethora of activity to study such phenomena in various experimental platforms. Specifically cold atom platforms, which can control interaction strengths and effective dimensionality, prove useful tools for studying such physics via the use of artificial gauges [2,3]. These artificial gauges induce desirable properties of charged particles in a magnetic field in charge neutral platforms - required to mimic the quantum Hall effect. Synthetic dimensions are one such powerful tool [4] which also construct an additional spatial dimension. Here we discuss a theoretical investigation of a harmonic synthetic dimension [5], in cold atoms, which has a tunable length and edge - perfect for studying topological edge-states of quantum Hall like systems. This investigation is working in tandem with an experiment in the University of Birmingham which hopes to realise these edge-states in the harmonic synthetic dimension. This is an extension of previous work inducing 1D Bloch oscillations in the harmonic synthetic dimension [6].

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Sr3LiIrO6: a potential quantum spin liquid candidate in quasi-1-D d4 iridate family

Dr Abhisek Bandyopadhyay[1,2], Dr Atasi Chakraborty[3], Prof Carlo Meneghini[4], Dr G B G Stenning[1], Dr Devashibhai Adroja[1], Prof Clemens Ritter[5], Prof Fabrice Bert[6], Prof A. V. Mahajan[7], Prof Sugata Ray[2]
[1]ISIS Neutron and Muon Source, STFC, Rutherford Appleton Laboratory, United Kingdom [2]School of Materials Science, Indian Association for the Cultivation of Science, India, [3]School of Physical Sciences, Indian Association for the Cultivation of Science, India, [4]Dipartimento di Scienze, Universita Roma Tre, Italy, [5]Institut Laue-Langevin, France, [6]Universite Paris-Saclay, CNRS, Laboratoire de Physique des Solides, France, [7]Department of Physics, Indian Institute of Technology India

Here we present a detailed study on an apparently isolated 2H- hexagonal spin-chain d^4 iridate Sr_3LiIrO_6 (SLIO) with geometrical exchange frustration. Our x-ray and neutron diffraction studies clearly reveal perfect Li-Ir chemical order along with desired stoichiometry in this compound, while x-ray absorption and x-ray photoemission spectroscopic investigations establish pure 5+ valence of Ir. We infer a magnetic ground state with finite Ir5+ magnetic moments, contrary to the anticipated nonmagnetic J=0 state, through combined dc susceptibility, ^{7}Li nuclear magnetic resonance (NMR), muon spin relaxation (μSR) and ab-initio electronic structure studies. Furthermore, our dc, ac magnetic susceptibilities (χ), neutron diffraction, NMR, μSR, magnetic heat capacity, and spin-polarized density functional theory (DFT) results unravel that despite having noticeable antiferromagnetic correlation among the Ir5+ local moments, this system evades magnetic ordering down to 0.05 K at least due to geometrical exchange frustration, arising from the comparable nearest- and next-nearest-neighbor interchain Ir-O-O-Ir superexchange interaction strengths with opposite signs. On top of it, our zero-field (ZF) μSR analysis shows coexistence of frozen spin dynamics with an overall fluctuating strongly correlated liquid-like magnetic state till down to the lowest measured temperature of 1.7 K. Finally, the linear T-dependence of the magnetic specific heat together with finite γ-term in both the zero and applied magnetic fields in the 0.05-4 K range, plus the power-law dependency of the NMR spin-lattice relaxation rate, suggest gapless spin-excitations from a metal-like spinon density of states in the magnetically disordered ground state of Sr_3LiIrO_6

SquidLab - a user-friendly program for background subtraction and fitting of magnetization data

Dr Matthew Coak[1,2,3], Mr Cheng Liu[4], Dr David Jarvis[4,5], Seunghyun Park[6,7], Dr Matthew Cliffe[8], Dr Paul Goddard[3]

[1]London Centre For Nanotechnology, University College London, London, United Kingdom, [2]Department of Physics and Astronomy, University College London, London, United Kingdom, [3]Department of Physics, University of Warwick, Coventry, United Kingdom, [4]Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom, [5]Institut Laue-Langevin, Grenoble, France, [6]Centre for Correlated Electron Systems, Institute for Basic Science, Seoul, Republic of Korea, [7]Department of Physics and Astronomy, Seoul National University, Seoul, Republic of Korea, [8]School of Chemistry, University of Nottingham, Nottingham, United Kingdom

We present an open-source program with full user-friendly graphical interface for performing flexible and robust background subtraction and dipole fitting on magnetization data. For magnetic samples with small moment sizes or sample environments with large or asymmetric magnetic backgrounds, it can become necessary to separate background and sample contributions to each measured raw voltage measurement before fitting the dipole signal to extract magnetic moments. This then allows a huge range of measurements that were not previously feasible to be easily carried out.

Originally designed for use with pressure cells on an MPMS3 magnetometer, SquidLab [1] is a modular object-oriented platform implemented in Matlab with a range of importers for different widely-available magnetometer systems and has been tested with a broad variety of background and signal types. The software allows background subtraction of baseline signals, signal preprocessing, and performing fits to dipole data. A plugin system allows users to easily extend the built-in functionality with their own importers, processes or fitting algorithms.

With close to 1000 downloads so far to a rich variety of labs worldwide, SquidLab is proving an indispensable tool for high-pressure magnetic measurements and a whole host of other applications. It is available for free under academic license – simply search for ‘Squidlab Warwick’ and download from Warwick’s WRAP archive service.

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Free induction decay processes of folded longitudinal acoustic phonons dependent on a constituent layer ratio in one period of GaAs/AlAs superlattices in a finite system: Effects of the phonon dispersion curve

Dr. Hideo Takeuchi[1,2]

[1]Division of Physics and Electronics, Osaka Metropolitan University, Osaka, Japan, [2]Faculty of Science and Technology, Sophia University, Chiyoda-ku, Japan

In the research field of quantum computing technology, coherence time is an essential factor of realizing practical systems. For example, Park et al. succeeded in maintaining coherence between the nuclear spin states on a time scale of 1 second in ultracold 23Na40K molecules [1]. In their work, hyperfine states was prepared in a crossed optical dipole trap at a temperature of about 300 nK, which strongly suppress free induction decay processes. In the free induction decay, when there is a distribution of dipole frequencies caused by fluctuations, the sum of the electromagnetic wave generated from the dipole ensemble decays with time evolution, even though the motion of each dipole does not decay. We note that, in quantum materials such as semiconductor superlattices, the dispersion relation influences the distributions of the eigenfrequency of quanta through the wavevector even at the absolute temperature of zero Kelvin. Accordingly, it is meaningful to investigate the relation between the free induction decay and dispersion relation. In the present work, we investigated the relation between the dispersion curve and the free induction decay of the folded longitudinal acoustic (FLA) phonon coherently generated by impulsively optical excitation. We performed a thought experiment, the Raman scattering measurement in the forward scattering configuration with use of the femtosecond laser pulses. The model sample structures were (GaAs)m/(AlAs)20-m superlattices with the total number of periods of 20, where the index m corresponds to the atomic layer thickness of 0.283 nm. In the thought experiment with numerical calculation taking account of the relaxation of the wave-vector conservation, the free induction decay time strongly depends on the dispersion relation. This phenomenon originates from the fact that the dispersion curve around the wave vector k ~ 0 strongly is strongly modified by the constituent layer of a single period, which reflects the gap width of the dispersion curves at k = 0. Accordingly, the design of the dispersion curve is an important factor for controlling the free induction decay.

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Suppressing superconductivity in high-Tc cuprates with intense current pulses

Mr. Tim Huijbregts[1,2], Ms. Caitlin M. Duffy[2], Mr. Bence Bernáth[2], Mr. Sven Badoux[2,3], Mr. Nigel E. Hussey[1,2]
[1]H.H. Wills Physics Laboratory, University of Bristol, Bristol, United Kingdom, [2]High Field Magnet Laboratory (HFML-EMFL) and Institute for Molecules and Materials, Radboud University, Nijmegen, Netherlands, [3]LNCMI-EMFL, CNRS UPR3228, Univ. Grenoble Alpes, Univ. Toulouse, INSA-T, Toulouse, France

Knowledge of the underlying (non-superconducting) ground state of high-Tc cuprates is key to understanding the origins of superconductivity. This is particularly important in the vicinity of the critical hole-doping p* at which the pseudogap closes, since the nature of the electronic state near p* provides a stringent test for many existing theoretical models. It is therefore desirable to suppress superconductivity in the vicinity of p* and study the electronic ground state that emerges. Unfortunately, this is precisely the regime where superconductivity is strongest with upper critical fields Hc2 that far surpass 100 T; field strengths beyond those available in state-of-the-art high field facilities. One solution to this problem is to suppress Hc2 by applying current densities close to the critical current density of the cuprate under study in combination with the maximum fields available at such a facility. To this end, a pulsed current system has been developed at HFML-EMFL that is able to generate current densities of the order of 10^6 - 10^7 A/cm^2. These intense current pulses can be as short as 5 μs, thereby minimising the effect of self-heating which drives the system away from the ground state when one applies a large DC current density [1]. By recording the waveforms of various elements in the electrical circuit, the behaviour can be both qualitatively and quantitively investigated. We thereby show that the combination of high magnetic fields and intense current pulses is a viable route to suppress superconductivity near p* and access the underlying non-superconducting electronic state.

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Quantum bath suppression in a superconducting circuit by immersion cooling

Dr Marijn Lucas[1], **Mr Nathan Eng[1]**, Dr Andrej Danilov[3], Dr Lev Levitin[1], Dr Aditya Jayaraman[3], Dr Andrew Casey[1], Dr Lara Faoro[4], Professor Alexander Tzalenchuk[1,2], Professor Sergei Kubatkin[3], Professor John Saunders[1], Dr Sebastian de Graaf[2]

[1]Royal Holloway University Of London, Egham, United Kingdom, [2]National Physical Laboratory, Teddington, United Kingdom, [3]Chalmers University of Technology, Goteborg, Sweden, [4]Google Inc., Venice, USA

The measured properties of superconducting quantum circuits appear to plateau out far above the dilution refrigerator base temperature, under usual thermalization schemes. This is reflected in the thermal state population of qubits, excess numbers of quasiparticles, and polarization of surface spins– factors contributing to reduced coherence.

Here we have studied a superconducting resonator immersed in liquid 3He [1], cooled by a cryogen-free adiabatic nuclear demagnetization refrigerator [2]. Electron spin resonance of surface atomic hydrogen demonstrates cooling to below 10 mK. The spectral density of low frequency noise is studied from 300 mK to below 1 mK. Down to just below 100 mK the noise increases with decreasing temperature, consistent with the predictions of the generalised tunnelling model of two level systems/two level fluctuators (TLS/TLF), and previous experimental work. Remarkably however, we observe that from 80 mK to the lowest temperatures the noise decreases; at 1 mK it is more than three orders of magnitude smaller than expected. Furthermore, measurements of resonator Q demonstrate a dramatic increase in power required to saturate the TLS.

These results demonstrate not only cooling by liquid 3He immersion, but also significant coupling between the 3He and the quantum bath of TLS/TLF. The fermionic quantum liquid 3He supports quasiparticle excitations and collective excitations: zero sound and spin fluctuations. Furthermore there is a magnetic surface boundary layer of solid 3He. The coupling mechanism to TLS/TLF remains an open question at this time. The demonstrated ability to both cool and reduce noise potentially opens a new route for understanding and mitigating decoherence in quantum processors.

The research leading to these results has received funding from the European Union's Horizon 2020 Research and Innovation Programme, under Grant Agreement no. 824109, European Microkelvin Platform.

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Exploring quantum paraelectricity as a mechanism for parametric amplification

Deepanjan Das[1], Edward Laird[1]
[1]*Lancaster University, Lancaster, United Kingdom*

Detecting galactic axions could solve one of the greatest challenges in physics, the identification of dark matter. This requires cutting-edge quantum electronics and highly advanced measurement techniques. In a strong magnetic field axions decay into photons resulting an extremely weak electromagnetic signal. To measure such tiny signal, a low noise amplifier which can be operated in an external magnetic field, is highly desirable to meet the standard quantum limit. We are developing such an amplifier for the QSHS axion search experiment [1].

This poster will describe how the resonance frequency of a superconducting resonator could be tuned in a controlled way by an external electric field. We have fabricated aluminium coplanar resonators on quantum paraelectric substrates (i.e. strontium titanate, potassium tantalate). The resonance frequency depends on the dielectric constant of the substrate. As a special feature of the paraelectric material, its dielectric constant changes in the presence of an external electric field [2]. We have applied dc voltage on the resonator to modify the capacitance and therefore the resonance frequency of the coplanar waveguide resonator. We are planning to characterise this resonator as a parametric amplifier by driving the system into the nonlinear regime by introducing a pump signal of the right frequency and power.

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Enhanced collection efficiency from single colour centres in aluminium nitride micropillars

Mr Huseyin Bilge Yagci[1,2], Dr Sam G. Bishop[1,2], Mr Joseph K. Cannon[1,2], Dr John P. E. Hadden[1,2], Prof. Anthony J. Bennett[1,2]

[1]Translational Research Hub, Cardiff University, Cardiff, United Kingdom, [2]School of Engineering, Cardiff University, Cardiff, United Kingdom

III-nitrides are a technologically important class of compound semiconductors that have formed the basis for the lighting and display applications around the turn of the century. Their wide and direct bandgap is tunable via alloying, and they have mature growth processes. Additionally, III-nitrides were hypothesized to host defects with quantum-mechanical emission statistics, giving them potential applications in quantum sensing and quantum communications. Recently, anti-bunched emission from isolated emitters within commercial AlN thin films in ambient conditions had been observed, albeit with a broad spectrum. Unfortunately, photon extraction efficiency from emitters within the host is limited by total internal reflection at the AlN-air interface.

Here, we show that the photon collection efficiency can be improved by fabricating micron-scale pillars around the emitters. The emission from an emitter at the centre of the micropillar and the total coupling to the collection optics with a numerical aperture of 0.9 is simulated via a commercial finite difference time-domain electromagnetic solver. The simulation results show that the photon collection efficiency to the collection objective at the zero-phonon line of the emitter can be increased by one order of magnitude, from 5.4% in the initial case to 51.9% for a maximally aligned emitter at the center. The optimized geometry is fabricated via a standard spinning -exposure - liftoff - dry etch process flow. We measure the autocorrelation histogram for a single emitter in a pillar using the Hanbury-Brown and Twiss apparatus, confirming the antibunched photon statistics consistent with the presence of a single quantum emitter.

Rapid Prototyping of Novel Devices with In-situ Deposition, Imaging and Thermal Nanolithography

Dr Arthur Coveney[1], Professor Kelly Morrison[1]
[1]*Loughborough University, Loughborough, United Kingdom*

As part of an EPSRC Strategic Equipment investment (EP/W006243/1) we will be installing a state-of-the-art thin film deposition, thermal scanning probe nanolithography and characterisation system that will consist of 3 parts:

1) Sputtering and e-beam chambers for precisely controlled deposition of metallic films, and reactive deposition of, for example, nitride or oxide thin films.

2) State-of-the-art thermal scanning probe lithography (T-SPL) – the NanoFrazor [1] - housed in a glovebox for nanolithography, heat assisted physical property modification and topography characterisation.

3) Scanning tunnelling and atomic force microscopy (STM/AFM) for local electronic structure and topography characterisation.

All 3 parts will be connected via common distribution chamber. Therefore interchanging a sample without exposing to air will be possible, with separate loadlocks on each part facilitating sample loading/unloading at each stage. This arrangement enables complete device preparation and characterisation without removing to air – a critical feature for artificial engineering of quantum properties using 2D materials.

To encourage a diverse user base we will be providing 'free at point of access' sessions for potential users, which will include specific training on the NanoFrazor and invite applications for this time. This poster will outline the features of the new equipment and the access route for external users.

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Euler class for topological phase transition of nodal lines in spring-mass systems

Sang Soon Oh[1], Haedong Park[1]
[1]*Cardiff University, Cardiff, United Kingdom*

The prime example of topological effects is topologically protected surface states due to the peculiar topology of energy bands or a dispersion relation, for instance, point degeneracy in a two-band system called the Dirac or Weyl points. In general, band structures can have different types of degeneracy such as nodal lines. Additionally, the topology of these nodal lines involves more than two bands at the same time, which is called a multigap topology. In this work, we theoretically demonstrate phase transitions of nodal lines in a multigap system using a classical spring-mass system. First, using the concept of frame-rotation charge, we show that nodal lines can have non-Abelian charges. Next, we prove that, if two adjacent nodal lines by the same pair of bands have the same (opposite) charges, they are stable (can be pair-annihilated). By tuning the spring constants, one degeneracy is braided around another in different band gaps, flipping its sign. Finally, to analyse the phase transition of nodal lines, for example, from two nodal lines to a nodal link, we employ the Euler class that is a topological invariant of many band systems.

Vibrating carbon nanotubes: A nanomechanical probe to study quantum phenomena in superfluid 3He/4He

Ms Saba Khan[1], Prof Edward Laird[1]
[1]*Lancaster University, Lancaster, United Kingdom*

Superfluid 3He/4He are one of the most fascinating systems in condensed matter physics. As a fermionic quantum fluid, 3He shares a range of features with unconventional superconductors, neutron stars, and possibly even the early universe – certainly at least the present one [1]. Therefore, by studying this fermionic system, we can hope to gain a better understanding of high-Tc superconductivity, the dynamics of topological defects, and cosmology.
Despite recent advances in nano-electro-mechanical technology [2], there is no developed technique to probe superfluids at a mesoscopic length scale. However, carbon nanotube nanomechanical resonators provide a new route to study mesoscopic systems such as superfluid 3He/4He. The mechanical vibrations are influenced by adsorbed masses, charges and impurities which can tune the resonant frequency of the resonator up to the energy required for quasiparticles formation ~70 MHz [3, 4].
This poster describes a proposal to measure superfluid helium3He/4He by immersing a vibrating carbon nanotube. By measuring the vibration frequency, we will infer how much of the surrounding fluid is clamped to it; by measuring the dissipation, we will infer the rate of quasiparticle dissipation; by measuring fluctuations in both quantities, we may learn about the dynamics of superfluid vortices.

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Quantum oscillations of a candidate bulk Dirac system

Ms. Ioana Paulescu[1], Mr Ylias Sadki[1], Mrs Amalia Coldea[1]
[1]*University of Oxford, Oxford, United Kingdom*

Quantum oscillations is a powerful technique for probing Fermi surface topography. Damping terms provide insight into the quasiparticle orbit parameters and phase factors of different orbits could access their origin and test any topological signatures. This work investigates the potential Dirac material BaGa2 via quantum oscillations by carrying out torque magnetometry measurements in fields up to 16T and temperatures down to 2K. The geometry of the Fermi surface pockets is mapped out by studying the angular dependence of the signal in magnetic field and extremal orbit parameters are determined by fitting to the Lifshitz-Kosevich formalism. The four fundamental frequencies discovered and their associated orbit parameters follow trends in broad agreement with both literature and density functional theory (DFT) calculations in WIEN2k. Phase analysis can be used to identify the presence of Berry phases, which acquire special values in orbits enclosing Dirac points of linear dispersion. The extracted phases could originate from topologically trivial bands, but employing different methods of extraction sheds light on the reliability of Berry phase detection.

Dynamical correlations in the Hubbard ladder after a pump-probe quantum quench

Elie Merhej[1], Robert Konik[2], Andrew James[1]
[1]*The Open University, Milton Keynes, United Kingdom,* [2]*Brookhaven National Laboratory, Upton, New York, USA*

State-of-the-art synchrotron facilities with femtosecond free electron X-ray lasers allow for ultrafast, time resolved, 'pump-probe' studies of quantum matter. These trRIXS experiments investigate out-of-equilibrium collective phenomena by first pumping a strongly correlated condensed matter system, and then probing the resulting correlations as a function of time.

We present density-matrix-renormalization-group (DMRG) and time-evolving-block-decimation (TEBD) results for the dynamical correlations in a half-filled Hubbard ladder subjected to a simulated laser pump. We find that the pump produces doublons which persist in the system and disrupt antiferromagnetic correlations. We also note the differences when the pump is applied along the legs of the ladder or along the rungs.

Unlocking the Hidden Power: Unravelling Sub-Bandgap Photoconductivity in Synthetic Cu2O under Pulsed Laser Excitation at IR wavelength.

Aisha Albeladi[1,2], Stephen Lynch[1], Chris Hodges[1], Craig Allford[1]
[1]*School of Physics and Astronomy, Cardiff, United Kingdom,* [2]*Department of Physics, College of Sceince and Art, KAU, Rabigh , Saudi Arabia*

Rydberg excitons are quantum quasi-particles found in solid-state materials such as cuprous oxide (Cu2O) and have potential applications, as spatially localised single photon sources [1]. To date, the observation of high principal quantum number excitons in naturally occurring gemstone material (n = 25,[2]) is yet to be replicated in the best performing synthetic Cu2O (n=10). The large spatial extent of high-n exciton wavefunctions makes them sensitive to defects within the Cu2O crystal lattice [3]. Therefore, the understanding and assessment of material quality is essential to further developing and exploiting this potential.

In this work we have developed a room-temperature high-resolution photoconductivity measurement to address sub-bandgap defect states in Cu2O. A wavelength tunable nano-second pulsed laser was used to illuminate the crystal between (710-1500 nm) and between Au Ohmic contacts deposited via thermal evaporation. Illumination of the device generates a photovoltage transient, (Figure 1) where two distinct timescales are observed. This transient photoresponse is attributed to two different response mechanisms and named the 'fast' and 'slow' responses, shown in red and blue respectively. Integration and subsequent data processing of the measured signal was performed as a function of wavelength and the resultant photoresponse spectra are displayed in Figure 2.

We observe several sharp spectral features in the photoconductivity spectrum which can be associated with sub-bandgap defects. The observed sub-bandgap features occur at coincidental wavelengths in both the fast and slow response spectra. These sub-band gap features are not normally visible in conventional spectroscopy techniques due to the lower dynamic range of the measurements. We have therefore demonstrated a powerful technique for material quality characterisation at room temperature, avoiding the need for time-consuming and expensive low temperature measurements.

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Modelling of Microstructure Evolution During Polymer Crystallisation

Rasha Algethami[1], Nigel Clarke[2]
[1]*The University of Sheffield , Sheffield, United Kingdom,* [2]*The University of Sheffield , Sheffield, United Kingdom*

We are developing phase-field models in which the molecular detail is coarse-grained into an order parameter that describes the local density of crystal or liquid. The phase-field model is then coupled to the Stokes equation of motion for fluid flow, assuming low Reynold's number. We are using a new approach to the modelling, known as fluid-particle dynamics, in which we treat the crystal as a high viscosity liquid rather than a solid. A series of two-dimensional numerical simulations were performed to investigate the rotation behaviour of the melt-crystal interface in rhombus polymer crystal at various values of interfacial energies, interfacial thickness, and angle between rhombus faces. Furthermore, the role of hydrodynamics in polymer crystal growth was studied when a single polymer crystal rotated during growth with anisotropic interface energies and varies interface thickness. In addition, comparison studies were carried out for the growth of the crystal during rotation when the interfacial thickness varied with time and when it remained constant. These simulations show that crystals rotate more when the width of the interface is thicker. Furthermore, single polymer crystals grow more during rotation with a fixed interface thickness.

Statistical Analysis of the Distribution of single atoms and Nanoclusters on Surfaces

Hanan Alhabeadi[1,2], Dr Wolfgang Theis[1]
[1]*School of Physics and Astronomy, University of Birmingham, Birmingham, United Kingdom,* [2]*Department of Physic, College of Science and Art, Saudi Arabia*

Studying the behaviour of single atoms and metal clusters on surfaces is highly interesting as it can be employed in many fields, such as catalysis, material science, and surface physics. This study examines the behaviour of single atoms and metal clusters on substrates using aberration-corrected transmission electron microscopy (AC-STEM) to explore and analyse their statistical distribution on the substrate.
A mass-selected cluster source was employed to prepare samples on two representative carbon substrates on TEM grids: a homogeneous substrate (amorphous carbon) and a non-homogeneous substrate (holey carbon). These samples are imaged by annular dark field (ADF)-STEM at atomic resolution. Python scripts are used to extract atom and cluster positions. These positions are used to calculate the nearest-neighbour distances (NND) between atoms and resulting statistical quantities, such as the NND probability density and cumulative distribution functions. These are visualised by histograms and kernel density estimation plots. The statistical data is compared to that of simulated data for random and selected biased distributions of atoms and clusters on a substrate in order to draw quantitative conclusion regarding the properties of the experimental data.

Superconductor/ferromagnet van der Waals heterostructure: Appearance of Majorana zero mode

Chandan Singh Chandan Singh[1,2]
[1]University of Birmingham, United Kingdom, [2]Indian Institute of Science Education and Research (IISER), India

Emerging quantum states may appear when two materials with different quantum states are brought in close proximity [1-2]. One promising system for exploring these states is the superconductor/ferromagnetic van der Waals (vdW) heterostructure, which is believed to be a cleaner system for investigating Majorana zero-energy modes [3-4]. In this context, we investigate a two-dimensional (2D) superconductor NbSe2, ferromagnetic insulator CrI3, and their vdW heterostructure using first-principles density functional theory calculations and Hamiltonian modelling. Our calculations accurately reproduce the electronic and magnetic structures of individual NbSe2 and CrI3 monolayers. In the vdW heterostructure, the proximity effect induces a finite magnetic moment, and the magnetic layer influences the spin-splitting of NbSe2 at the valley points. We modelled this heterostructure using a low-energy tight-binding Hamiltonian of NbSe2 supplemented with an external magnetic field term using the Bogoliubov-de Gennes Hamiltonian. In the superconducting state, we observed the emergence of six pairs of nodal points within the hexagonal Brillouin zone under an applied in-plane magnetic field. Furthermore, a Majorana flat band appears on the armchair edge of the NbSe2 nano-ribbon, while it disappears on the zigzag edge. Our findings suggest that the vdW SC/FM heterostructures hold great promise for exploring emerging quantum states, specifically Majorana zero-energy modes.

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