Plenary Talks

Using uniaxial pressure to both tune and probe quantum materials

Andrew Mackenzie[1]
[1]*Max Planck Institute for the Chemical Physics of Solids, Germany*

Plenary Speaker: Professor Andrew P Mackenzie, July 5, 2024, 09:00 - 10:00

In this talk I will discuss rapid developments, taking place over the past decade or so, in applying uniaxial pressure to quantum materials using piezo-activated vices. In the first stages of using the new experimental capabilities, the focus was on applying large static uniaxial pressures, up to 3 GPa so far, to generate large changes in the physical properties of unconventional superconductors and magnets. The vice provided the tuning of the properties, which were probed by other techniques such as electrical resistivity or magnetic susceptibility. Only more recently has it become clear that exquisitely precise thermodynamic information can be obtained from simultaneously probing the elastic response of the materials to the applied pressure. These new techniques rely on combining static pressure with a tiny oscillatory component, and locking in to the responses of the material at the frequency of those oscillations. They are enabled only via the basic strategy of applying the pressure using piezoelectric actuators. In my opinion an entirely new avenue of quantum materials research can be opened with this new combination of tuning and measurement, as I will attempt to explain.

Exploring the Atomic Structure and Dynamics of 2D Heterostructures with Advanced Electron Microscopy

Prof Sarah Haigh[1], Dr Nick Clark, Dr Astrid Weston, Dr Rui Zhang, Dr Yi-Chao Zou, Prof Roman Gorbachev
[1] *University Of Manchester, United Kingdom*

Plenary Speaker: Professor Sarah Haigh, July 4, 2024, 16:30 - 17:30

Atomic structure of surfaces and interfaces is key to the performance of 2D materials and their heterostructures including for exploring new optoelectronic phenomena and quantum behavior. Scanning transmission electron microscopy (STEM) techniques are key for analysing this behaviour and we to investigate the behavior of moire superlattices in twisted transition metal dichalcogenide (TMD) heterostructures to uncover unusual lattice reconstruction and strong piezoelectric textures [1], which can be engineered by the application of applied field in the electron microscope [2]. Complementing imaging with scanning diffraction analysis (termed 4D STEM) and elemental mapping by energy dispersive x-ray spectroscopy (EDS) allows further investigation of larger scale atomic structure variations in 2D materials. We illustrate this by combined 4D STEM imaging and EDS spectroscopy analysis to reveal variability in intercalated TMD structures at the nanoscale and how these evolve during deintercalation as a function of time and annealing temperature [3]. Finally, I will discuss the use of 2D heterostructure liquid cells [4] for uncovering the dynamics of atomic species on the surfaces of 2D materials [5] where advanced image processing is being applied to allow quantitative understanding of atomic behaviour with statistically significant data sets of 10000-1000000 individual STEM measurements.

References

[1] A. Weston et al, Nature Nanotechnology, 15 592–597 (2020). [2] A. Weston et al, Nature Nanotechnology 17, 390–395, (2022). [3] S. Shao et al, Advanced Functional Materials, 33 2214390 (2023) [4] D. Kelly, et al, Advanced Materials, 33, 2100668, (2021), [5] N. Clark et al, Nature, 609, 942–947 (2022)

Multiferroicity and magnetoelectricity in the flatland

Dr. Silvia Picozzi[1]
[1]*CNR Spin, Italy*

Plenary Speaker: Dr. Silvia Picozzi, July 2, 2024, 09:00 - 10:00

Multiferroicity and magnetoelectricity (i.e. the coexistence and coupling between long-range magnetic and electric dipolar order) constitute two related landmark phenomena in quantum physics, where profound fundamental aspects (i.e. microscopic interactions between charge and spin degrees of freedom) are intimately related to technological milestones (multifunctional devices tuned by electric/magnetic fields). In this context, the reduction of dimensionality from 3D to 2D has been boosted by the recent discoveries of multiferroicity in NiI2 layers [1], obtained via a joint theory-experiments approach down to the single-layer limit. I will show several examples of first-principles modelling for multiferroic and magnetoelectric 2D-materials, including vanadium dihalide-monolayers and domain walls in CrI3 layers, highlighting the potentiality of cross-coupling phenomena in van der Waals materials.

References

[1] Song Q., Occhialini C.A., Ergecen E., Ilyas B., Amoroso D., Barone P., Kapeghian J., Watanabe K., Taniguchi T., Botana A., Picozzi S., Gedik N., Comin R., Evidence for a single-layer van der Waals multiferroic, Nature 602 (2022), 601.

Strongly correlated electrons in moire materials: an optical investigation

Dr. Atac Imamoglu[1]
[1]*ETH Zurich, Switzerland*

Plenary Speaker: Professor Ataç İmamoğlu, July 4, 2024, 09:00 - 10:00

Moire superlattices in two dimensional semiconductors have enabled the observation of a wealth of phenomena driven by strong electronic correlations, ranging from Mott-Wigner states to quantum anomalous Hall effect. In this talk, I will describe magnetic properties of van der Waals heterostructures forming a frustrated triangular lattice in the vicinity of Mott-insulator states of electrons. By directly measuring electronic magnetization through the strength of the polarization-selective attractive polaron resonances, we find that when the Mott state is doublon doped, the system exhibits ferromagnetic correlations in agreement with Nagaoka model. Our observations, which are supported by DMRG calculations, provide a direct evidence for magnetism with a kinetic origin.

Correlated Disorder in Functional Materials

Prof. Andrew Goodwin[1]
[1] *University of Oxford, United Kingdom*

Plenary Speaker: Professor Andrew Goodwin, July 3, 2024, 16:30 - 17:30

All materials are disordered at finite temperature. Sometimes that disorder is random; more frequently it is not. Our group is particularly interested in understanding cases where disorder is actually very strongly correlated, and these correlations are important for particular material properties. This talk will cover some of the key concepts of correlated disorder [1] and the experimental techniques that allow characterisation of disordered states [2]. It will draw on a number of recent examples from the group, including biominerals [3], metal-organic frameworks [4], and frustrated magnets [5].

[1] Simonov & Goodwin, Nat. Rev. Chem. 4, 657 (2020)
[2] Keen & Goodwin, Nature 521, 303 (2015)
[3] Nicholas et al., Nat. Chem. 16, 36 (2024)
[4] Meekel et al., Science 379, 357 (2023)
[5] Bulled et al., Phys. Rev. Lett. 128, 177201 (2022)

Coulomb interactions in organic semiconductors

Prof Richard Friend[1]
[1] *University of Cambridge, United Kingdom*

Plenary Speaker: Sir Richard Friend, July 2, 2024, 16:30 - 17:30

Pi-conjugated organic molecules and polymers now provide a set of well-performing semiconductors that support devices, including light-emitting diodes (LEDs) as used in smart-phone displays and lighting, field-effect transistors (FETs) and photovoltaic diodes (PVs). Semiconductor properties for the organics are however very different to traditional inorganic systems. In particular, dielectric screening is weak, so that Coulomb interactions between charges and associated spin exchange energies are big, often much larger than kBT. Management of transport and of excited state spin is fundamental for efficient LED and solar cells operation. I will discuss some of our recent work in Cambridge.

I will report in particular our recent work on spin radical organic semiconductors that can be used as efficient light emitters in LED devices, showing very high luminescent [1,2]. We have explored the use the radical semiconductor as the emissive 'guest' in a regular organic LED emissive layer 'host' where the radical semiconductor is able to harvest both singlet and triplet excitons formed in the host material [3]. I will also discuss on recent studies of photogeneration of high spin states in radical semiconductors. These include coupled doublet-triplet systems that evolve to quartets and quintets [4], and di-radical structures where both singlet and triplet spin states are optically accessible and luminescent. These provide opportunities for optical writing, manipulation and reading of spin states.

References

[1] Ai, X, et al. Nature 2018, 563, 540. DOI: 10.1038/s41586-018-0695-9.
[2] Ghosh, P, et al Nature 2024, DOI: 10.1038/s41586-024-07246-x
[3] Li, F et al Nature Communications 2022, DOI: 10.1038/s41467-022-29759-7.
[4] Gorgon, S, et al. Nature 2023, 620 (7974) DOI: 10.1038/s41586-023-06222-1.

Surface Science of Functional Oxides

Ulrike Diebold[1]
[1]*TU Wien, Austria*

Plenary Speaker: Professor Ulrike Diebold, July 3, 2024, 09:00 - 10:00

The arrangement of the top layer of atoms on a solid -- and the resulting electronic and chemical properties – affect and sometimes even dominate its functionality. In the talk, I will showcase how we can use basic physical phenomena – tunneling, diffraction, and change in resonance frequencies – to measure surface properties in an atom-by-atom fashion. Such experiments can be interlinked tightly with theoretical computations by investigating well-defined samples in a controlled environment. Examples include perovskite oxides, where surface polarity, polaron formation, and compensating defects all play a role, and where surface science techniques can help perfecting the epitaxial growth of thin films.

Invited Talks

Observation of a Kondo impurity state and universal screening using a charge pseudospin

C Piquard[1], P Glidic[1], C Han[2], A Aassime[1], A Cavanna[1], U Gennser[1], Y Meir[3], E Sela[2], **Anne Anthore**[1, 4], F Pierre[1]

[1]Université Paris-Saclay, France, [2]Tel Aviv University, Israel, [3]Ben-Gurion University of the Negev, Israel, [4]Université Paris Cité, France

Session: Spintronics, July 4, 2024, 10:30 - 12:40

The Kondo effect, deriving from a local magnetic impurity mediating electron-electron interactions, constitutes a flourishing basis for understanding a variety of intricate many-body problems. Its experimental implementation in tunable circuits has made possible advances through well-controlled investigations. However, these have mostly concerned transport properties, whereas thermodynamic observations - notably the fundamental measurement of the spin of the Kondo impurity - remain elusive in test-bed circuits.

In this talk, I will present how we directly observe the state of the impurity and its progressive screening with a novel combination of a "charge" Kondo circuit and a charge sensor. We establish the universal renormalization flow from a single free spin to a screened singlet, the associated reduction in the magnetization in the the impurity's residual entropy from k_B log(2) to 0.
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Superconductivity in graphene bilayers - New directions from proximity effect to unconventional pairing

Julien Barrier

Session: Tuning many-body interactions, July 4, 2024, 14:00 - 16:05

Since the isolation of graphene, significant efforts were made to induce superconductivity in graphene and related heterostructures. Early work focused on superconducting-graphene-superconducting junctions, which allowed for studying proximity superconductivity through high-mobility two-dimensional electron gases (2DEGs). This approach yielded results that surpassed those obtained with traditional 2DEGs. Recent advances have combined the quantum Hall effect with proximity superconductivity, holding great promise for both fundamental physics and metrology applications. More recently, superconductivity has been observed to spontaneously emerge when two graphene layers are twisted relative to each other, leading to band hybridisation and flattening. The exact mechanism behind this superconductivity remains a topic of ongoing debate.
My presentation will explore these two complementary directions through specific examples. First, I will discuss how domain walls in minimally twisted bilayer graphene enable exceptionally robust proximity superconductivity in the quantum Hall regime. This allows Josephson junctions to function in magnetic fields approaching the upper critical field of the superconducting electrodes [1]. Secondly, I will present an experiment that utilises the strong Coulomb interactions facilitated by van der Waals heterostructures. This experiment demonstrates that complete suppression of superconductivity in magic-angle bilayer graphene is possible through Coulomb screening, suggesting a non-conventional Cooper pairing mechanism [2].

[1] J Barrier et al, “One-dimensional proximity superconductivity in the quantum Hall regime”, Nature 624, 8009 (2024) [2] J Barrier et al, “Screening of superconductivity in magic-angle twisted bilayer graphene”, submitted (2024)

Extreme light-matter coupling: What happens when light is confined to the atom scale?

Professor Jeremy Baumberg[1]
[1] *University of Cambridge, United Kingdom*

Session: Polaritons 2 and cavity QED, July 2, 2024, 14:00 - 16:10

Our ability to trap light into extreme nanoscale gaps between coinage metals using plasmonics has enabled routine vibrational measurements of monolayers, even within active molecular electronics devices. Emitters in such nanogaps couple very strongly, switching to peculiar coherent states. I also show how plasmonically-enhanced light-induced van-der-Waals forces can pull single adatoms from metal facets with thousand-fold stronger optical forces. This creates 'picocavities' which confine light to volumes smaller than a single atom, allowing individual transient bonds to be seen, and molecules tracked in real time. Such spectroscopy reveals a wealth of information, from how voltages twist conducting molecules, to how catalysis operates at individual adatoms.

Interfacial electron-phonon coupling in 2D materials

Felix Baumberger[1]
[1] *Université de Genève, Switzerland*

Session: Tuning many-body interactions, July 4, 2024, 14:00 - 16:05

Hexagonal boron nitride (hBN), a polar wide gap insulator, is the gate dielectric of choice in the field of 2D materials. However, surprisingly little is known about how hBN affects the electronic properties of 2D materials of interest. Here, we use nano-ARPES to study the prototypical systems of monolayer transition metal dichalcogenide semiconductors on hBN. Our data show two replica bands of the semiconductor valley at energies close to hBN phonon modes. This is the fingerprint of long-range electron-phonon interaction across the interface. Our data is well reproduced by a generic model describing the propagation of a charged particle above a polar substrate, suggesting that interfacial electron-phonon coupling is universal for 2D materials encapsulated in hBN. Consistent with this interpretation, control experiments on non-polar graphite substrates do not show the replica bands observed on hBN.

Physics and Materials Science of Heavy Element Thin Films

Dr Christopher Bell[1]
[1] University of Bristol, United Kingdom

Session: Thin Films, July 5, 2024, 10:30 - 12:30

Thin films of heavy elements – in particular uranium – open up a wealth of interesting directions for both materials science and physics investigations. Much of the complexity is driven by the 5f electrons, which can show both itinerant or localized behaviour. In this talk I will first briefly describe the Facility for Radioactive Materials Surfaces in Bristol [1], and the range of studies it can carry out [2]. I will then focus on two particular topics. I will discuss a structural study of a topotactic phase transition in elemental uranium between an epitaxy-induced metastable hexagonal-close-packed phase, and the bulk groundstate orthorhombic structure [3]. Next I will discuss more recent work combining uranium with the conventional superconductor Nb to study the creation of novel types of superconductivity [4].

[1] https://nnuf-farms.bristol.ac.uk/
[2] Springell et al., Advances in Physics 71, 87 (2022)
[3] Nicholls et al., Phys. Rev. Materials 6, 103407 (2022)
[4] Hussain et al., (in preparation)

Charge Order in Cuprate Superconductors

Antony Carrington[1]
[1] *University of Bristol, United Kingdom*

Session: Superconductivity 1, July 2, 2024, 14:00 - 16:00

Charge order has been found in different parts of the phase diagram in various cuprate high temperature superconductors. Originally, found only close to a doping of p=0.12, it is now known to exist, in different forms, over a wide region of the underdoped part of the phase diagram as well as in the overdoped part for some materials. In this talk I will discuss how the charge order affects transport properties, and how this is affected by parameters such as pressure, strain and disorder. I will present x-ray and transport studies of the influence of controller point disorder on the charge order in underdoped YBa2Cu3O6+x. The surprising result is that a relatively high level of disorder has minimal affect on the charge order despite destroying the superconductivity.

Manipulation and transport of excitons in monolayer semiconductors and 2D antiferromagnets

Alexey Chernikov[1]
[1]TU Dresden, Germany

Session: 2D materials 2, July 4, 2024, 14:00 - 16:00

Two-dimensional transition metal dichalcogenides offer an excellent platform to study non-linear dynamics of tightly-bound exciton quasiparticles. The properties of the excitons and their optical response change drastically in the presence of free charges, leading to emergence of many-body states described as trions or Fermi polarons. The physics of such Bose-Fermi quasiparticle mixtures have attracted a lot of interest in the scientific community and motivated the development of methods to control them on ultrafast time-scales. In addition, excitons were recently demonstrated to play central role also for magnetic 2D materials, with open questions regarding exciton mobility and its relation to the magnetic order, from both fundamental and technological perspectives.

The first part of the talk will be focused on the use of intense THz pulses to transiently modify light-emission of exciton-electron ensembles in monolayer semiconductors. We demonstrate a near complete, THz-induced trion-to-exciton conversion by monitoring time resolved photoluminescence after optical excitation. It offers new pathways to manipulate exciton-electron mixtures, triggering a non-linear optical response by low-energy photons on picosecond timescales. In the second part, I will discuss exciton transport in the layered semiconducting antiferromagnet CrSBr. Strong influence of the magnetic order on the exciton propagation will be discussed including rapid, non-linear exciton expansion in ultra-thin layers as well as contraction of the exciton clouds at low temperatures. These results are particularly interesting in the context of magnetic control of exciton transport and the consequences of coupling optical excitations to the magnetic order.

Extracting spin from an antiferromagnet at picosecond timescales

Chiara Ciccarelli
[1] *University of Cambridge, United Kingdom*

Session: Magnetism 2, July 2, 2024, 14:00 - 16:00

Interfaces in heavy metal– antiferromagnet heterostructures have recently become highly investigated and debated systems in the effort to create spintronic devices that function at terahertz frequencies. Such heterostructures have great technological potential because antiferromagnets can generate sub-picosecond spin currents which the heavy metal can convert into charge signals. In this talk I will present our recent work on the optically induced picosecond spin transfer from antiferromagnets to Pt using time-domain THz emission spectroscopy. We will focus on two studies in antiferromagnetic insulators KCoF3 and KNiF3, and in antiferromagnetic metal FeRh. Through our studies, we are able to shine light on the microscopy of spin transfer at picosecond timescales and identify key figures of merit for its efficiency. Our results are important for progressing in the fundamental understanding of the highly discussed physics of the heavy metal/antiferromagnet interfaces, which is the necessary cornerstone for the designing of femtosecond antiferromagnetic spintronics devices with optimized characteristics.

Quantum oscillations of superconducting iron-chalcogenides FeSe1-xSx

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

Session: Superconductivity 3, July 4, 2024, 10:30 - 12:40

Iron-chalcogenides superconductors display intertwined electronic nematic and spin-density wave phases and their role in superconducting pairing is difficult to assess. However, versatile tuning parameters, like applied pressure and chemical pressure [1,2], can be used to separate and explore their relative importance. In my talk, I will present quantum oscillations studies in FeSe1-xSx using magnetotransport and tunnel diode oscillator experiments tuned both by chemical and applied pressures [3,4,5,6]. I will discuss the evolution of the Fermi surface and the quasiparticle effective masses in the high-pressure phase of the tetragonal FeSe1-xSx where superconductivity is enhanced. These findings will be compared with magnetotransport studies to understand the signatures of different competing electronic phases with superconductivity [7].

References

[1]. A. I. Coldea, Frontiers in Phys. 8, 594500 (2021).
[2]. A. I. Coldea et al., npj Quantum Materials, 4, 2 (2019).
[3]. P. Reiss et al, Nature Physics, 16, 89 (2020).
[4]. P. Reiss et al, Phys. Rev. Lett. 127, 246402 (2021)
[5]. Z. Zajicek et al., A. I. Coldea, Phys. Rev. Res. 4, 043123 (2022).
[6]. Z. Zajicek et al., A. I. Coldea, accepted (2024).
[7]. P. Reiss et al, arXiv.2212.06824 (2022).

Dispersion of flat-bands at the 1T-termination of 4Hb-TaS2 probed by quasiparticle interference

Carolina de Almeida Marques[1], Berk Zengin[1], Aleš Cahlík[1], Helmuth Berger[2], Ana Akrap[3], Fabian Natterer[1]
[1]University of Zurich, Switzerland, [2]École Polytechnique Fédérale de Lausanne, Switzerland, [3]University of Fribourg, Switzerland
Session: 2D Materials 1, July 3, 2024, 10:30 - 12:40

The interplay between adjacent layers in heterostructures of van der Waals materials leads to rich phase diagrams with a wide range of strongly correlated electronic states, from Mott insulators to superconductors. The recent advent of twisted bilayer graphene added yet another tuning knob, with tiny changes to the twist angle between adjacent layers having a strong impact on the observed ground state. A natural heterostructure of alternating layers of 1T and 1H structural coordination is found in 4Hb-TaS_2. Individually, while 2H-TaS_2 is a superconductor coexisting with an incommensurate charge density wave (CDW), the 1T-TaS_2 is an insulator with a commensurate CDW. In 4Hb-TaS_2, we find that both surface terminations are metallic as probed by scanning tunneling microscopy. The angle between the unit cells of the CDWs in each adjacent layer leads to Moiré patterns and large unit cells. We show the bandwidth and the observation of chiral states as probed by quasiparticle interference on the 1T-terminated surface. We observe that within a broad energy range, the energy dispersion is indistinguishable between two CDW orientations, however, we find a flat band just above the Fermi level, whose degeneracy is lifted for one of the orientations. Our results show that the alignment between the CDWs on the topmost layers influences the low-energy electronic structure and further enriches the available tuning knobs in TaS2.

Jahn-Teller Distortions in NaNiO2

Sian Dutton[1]
[1]*University of Cambridge, United Kingdom*

Session: New Materials 2, July 2, 2024, 14:00 - 16:00

NaNiO2, and solid solutions with it as an end-member, have been studied as a Na-ion battery cathode material, and it exhibits a similar structure to other battery materials LiNiO2, α-NaMnO2, and LiMnO2. NaNiO2 is a layered structure derived from a cation-ordered rock-salt consisting of alternating layers of NaO6 and Jahn-Teller-active NiO6 edge-sharing octahedra below the Jahn-Teller transition temperature, TJT, where it is monoclinic. Above TJT where NaNiO2 is rhombohedral, diffraction measurements show the absence of a Jahn-Teller distortion from the average structure, though to our knowledge there have been no probes of the local structure. In this talk, I will present local probes as evidence for a displacive Jahn-Teller transition in NaNiO2. I will discuss neutron total scattering data (from which we analyse a pair distribution function using big box analysis), the extended x-ray absorption fine structure (EXAFS), and 23Na magic-angle spinning solid state nuclear magnetic resonance (NMR). I will present our results and present direct experimental evidence for a displacive transition with a suppression of the Jahn-Teller distortion at TJT, supported by ab initio molecular dynamics simulations. The results will be compared to the order-by-disorder Jahn Teller transition observed in LaMnO3. The changes in the Jahn-Teller transition in NaNiO2 under pressure and when isovalantly doped with Co will also be discussed.

Momentum dependent scaling exponents of cuprate strange-metal self energies: ARPES meets semi-holography

S Smit[1], E Mauri[2], L Bawden[1], F Heringa[1], F Gerritsen[1], E van Heumen[1], Y.K. Huang[1], T Kondo[3], T Takeuchi[4], N.E. Hussey[5,6], M Allan[7], T.K. Kim[8], C Cacho[9], A Krikun[9], K Schalm[10], H.C.T Stoof[2], **Mark Golden**[1,11]

[1]University of Amsterdam, Netherlands, [2]Utrecht University, Netherlands, [3]University of Japan, [4]Toyota Technological Institute, Japan, [5]Radboud University, Netherlands, [6]University of Bristol, United Kingdom, [7]Leiden Institute of Physics, Netherlands, [8]Diamond Light Source, United Kingdom, [9]KTH and Stockholm University, Sweden, [10]Institute-Lorentz for Theoretical Physics, Netherlands, [11]Dutch Institute for Emergent Phenomena, Netherlands

Session: Superconductivity 2, July 3, 2024, 14:00 - 16:10

ARPES enables the precise experimental determination of the electronic self-energy as we present here from the strange metal single-layer cuprate (Pb,Bi)2Sr2−xLaxCuO6+δ over a wide range in □- and T for k along the nodal direction. Constant energy cuts through the spectral function (MDCs) show a non-Lorentzian lineshape as k increases away from kF: the nodal self-energy is k dependent. These experimental data provide a new test for aspiring theories.

The self energy extracted from experiment is captured remarkably well by a power law that smoothly evolves with hole doping with - crucially - a k-dependent scaling exponent. In fact, this description emerges naturally from AdS/CFT-based semi-holography, putting a spotlight on holographic methods for the quantitative modelling of strongly interacting quantum materials like the cuprate strange metals [1].

[1] S. Smit et al., arxiv.org/pdf/2112.06576. Nature Communic ations: accepted for publication.

Spectroscopic-imaging scanning tunneling microscopy on quantum liquid crystals

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[1]RIKEN CEMS, Japan

Session: Magnetism 1, July 2, 2024, 10:30 - 12:40

Various electronic states that break rotational and translational symmetries of the underlying crystal lattice are often observed in close proximity to the unconventional superconducting phases in cuprates and iron-based superconductors. These “quantum liquid crystal” states have attracted much attention and can directly be investigated by spectroscopic-imaging scanning tunneling microscopy. We have developed ultra-low-temperature high-magnetic-field scanning tunneling microscopes to investigate the electronic states of various quantum liquid crystals and to search for as-yet-unknown quantum liquid crystals. We will describe recent results regarding the relation between nematicity and superconductivity in the iron-based superconductor FeSe and the pair density wave state in NbSe2.

Ultranodal state in multiband spin-1/2 superconductors

Prof. Peter Hirschfeld[1]
[1] *University of Florida, United States of America*

Session: Superconductivity 1, July 2, 2024, 14:00 - 16:00

Recent measurements on the tetragonal phase of the iron-based superconductor FeSe,S support the existence of a remarkable phase where the superconducting state manifests a finite residual density of states arising from patchlike nodal surfaces. This ``ultranodal" state, stable in the clean limit, can arise in situations where conventional intraband spin singlet pairing is highly anisotropic and coexists with time-reversal symmetry breaking interband spin triplet interactions. Here I present a microscopic scenario including ferromagnetic interactions that can account for nonunitary pairing and C4 symmetry breaking in the superconducting state that is also observed in recent experiments. Recent NMR experiments FeSe,S show upturns in spin-lattice relaxation at low temperatures, apparently due to spin fluctuation scattering between the Bogolibov Fermi surface sheets, but these are consistent with the theory only if electronic correlations are included.

Recent advances on quantitative theory for near-1D correlated systems in 2D and 3D

Dr. Adrian Kantian[1]
[1]*Heriot Watt University, United Kingdom*

Session: Electronic Structure 2, July 4, 2024, 10:30 - 12:30

For techniques based on matrix product states (MPS), entanglement scaling typically precludes working with large systems, while for Quantum Monte Carlo (QMC) methods the sign problems leads to exponentially growing errors as temperature is lowered.

In this talk I will provide an overview of recent developments that can circumvent the problem of entanglement-scaling in MPS-based methods for the near-1D class of 2D and 3D systems, i.e. systems for which coupling is much stronger in one direction that it is the other(s).
These new approaches are applicable to both fermions and bosons, for systems in equilibrium as well as as out-of-equilibrium ones, such as fusing MPS-techniques with mean-field or low-energy energy subspace expansion approaches.

With the resulting hybrid algorithms it is possible to study problems not previously amenable to many-body numerics. These range from deliberately designing 3D high-Tc model materials, to studying dynamically induced superconductivity and spin glasses on highly anisotropic triangular lattices.

Holstein polarons, Rashba-like spin splitting and Ising superconductivity in electron-doped MoSe2

Timur Kim[1]
[1] *Diamond Light Source, United Kingdom*

Session: Electronic Structure 1, July 3, 2024, 10:30 - 12:40

Interaction between electrons and phonons in solids is a key effect defining physical properties of materials such as electrical and thermal conductivity. In transitional metal dichalcogenides (TMDCs) the electron-phonon coupling results in the creation of polarons, quasiparticles that manifest themselves as discrete features in the electronic spectral function. In this study, we report the formation of polarons at the alkali-dosed MoSe2 surface, where Rashba-like spin splitting of the conduction band states is caused by an inversion-symmetry breaking electric field. In addition, we observe the crossover from phonon-like to plasmon-like polaronic spectral features at MoSe2 surface with increasing doping. Our findings support the concept of electron-phonon coupling mediated superconductivity in electron-doped layered TMDC materials, observed using ionic liquid gating technology. Furthermore, the discovered spin-splitting at the Fermi level could offer crucial experimental validation for theoretical models of Ising-type superconductivity in these materials.

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Spins in diamond for exploring quantum dynamics of interacting spin systems and for quantum sensing applied to life sciences

Dr Helena Knowles[1]
[1] *University of Cambridge, United Kingdom*

Session: Materials for Quantum Technologies 3, July 4, 2024, 14:00 - 16:00

Diamond-based quantum sensors that utilise the electronic spin of nitrogen-vacancy defects have applications in probing phenomena both in soft and solid-state systems. They promise advances in understanding the complexity of interacting quantum systems, and in developing new diagnostics and treatment technologies for healthcare.

In this talk, I will present our latest results on performing nanoscale quantum sensing in living cells for reporting two parameters simultaneously: temperature and viscosity.1,2,3 Temperature and viscosity are key parameters of interest that relate to cellular energetics and metabolism, morphological changes, cell division and active transport. The ability to correlate different parameters can help shed light on the development of cellular malfunction at the onset of a disease.

I will further discuss our recent work on enhanced nuclear spin initialisation in diamond, where we demonstrate how a recently developed pulsed protocol4 can provide advantages over more established techniques. This can support the realisation of highly controlled spin ensembles for probing quantum many-body effects in spin-based quantum simulator systems.

[1] S. Belser et al., Appl. Phys. Lett. 123 (2023) 020501
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[3] L. Shanahan et al., arXiv:2406.01181 (2024)
[4] O. Whaites et al., Phys. Rev. Res. 4, 013214 (2022)

Towards single polariton optical nonlinearity in semiconductor microcavities

Dmitry. N. Krizhanovskii[1]
[1]*The University of Sheffield, United Kingdom*

Session: Polaritons 2 and cavity QED, July 2, 2024, 14:00 - 16:10

Quantum platforms utilising photons as qubits are very promising for quantum computing, communication and imaging. The key challenge of quantum optical applications is the realisation of scalable systems enabling strong single-photon interactions through Kerr-like optical nonlinearity. Exciton-polariton systems based on 2D excitons in quantum wells or 2D materials may provide this combined nonlinearity and scalability [1] paving the way towards development of controlled phase shift gates [2], photon number detectors and sorters [3]. In my work I will review our experimental work revealing strong cross-phase-modulation between signal and control beams at few photon average intensities in the solid micropillar and tunable open access microcavity system [4], where strong nonlinearity is enabled by polariton lateral confinement (~1 μm) and high Q-factor (up to 30000). Phase shifts up to 80 mrad per polariton are observed, which already approaches those in photonic structures containing single photon emitters (single quantum dots or atoms). Our phase shift measurements correlate with the antibunching in the second order correlation function g(2)(0)~0.97 observed for the microcavity driven resonantly with a weak coherent beam. Perspectives in increasing the strength of polariton optical nonlinearity further using di-polaritons or Rydberg excitons will be also discussed [6].

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Spin dynamics of van der Waals magnets probed by superconducting resonators and electron doping in Cr2Ge2Te6

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Session: Spintronics, July 4, 2024, 10:30 - 12:40

Two dimensional (2D) layered van der Waals (vdW) materials can offer their unique physical properties due to their chemical bonding as well as low crystalline symmetry. The weak vdW bonding allows to mechanically exfoliate individual layers, down to one monolayer in many cases while maintaining thermodynamically stable layers [1]. When it comes to magnetism, this is a perfect material class to study the two dimensionality of magnetic ground states [2-3] and their dynamics and there have been a number of studies to reveal unique properties of vdW magnetic systems [4].
To establish the methodology of studying spin dynamics and magnetic fluctuations in the monolayer limit for vdW magnets, we are developing a microwave technique to efficiently couple magnons and photons down to that limit. To this end, we use on-chip superconducting resonators with a high quality-factor and small mode-volume to match nano-meter thick vdW flakes. By transferring Cr2Ge2Te6 flakes on superconducting lumped element NbN resonators, we achieve the collective coupling strength (rate) of 13 MHz to 18 nm thick Cr2Ge2Te6 [5]. The linewidth of the photon-magnon hybrid mode is used to analyse the magnetic properties of Cr2Ge2Te6. I will discuss more technical details as well as our strategy of how to achieve sensitive measurements of monolayer vdW magnets.
In the second part, I will also discuss spin-glass states generated in van der Waals magnet Cr2Ge2Te6 by Na intercalation [6]. A series of dynamic magnetic susceptibility measurements/analysis confirms the formation of magnetic clusters representing slow dynamics with a distribution of relaxation times. The intercalation also modifies other macroscopic physical parameters including the significant enhancement of TC from 66 K to 240 K and the switching of magnetic easy-hard axis direction.

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Electrons, excitons and phonons in moiré materials

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Session: 2D Materials 1, July 3, 2024, 10:30 - 12:40

Twisted multilayers of two-dimensional materials are a fascinating new class of quantum materials. By stacking and twisting two or more monolayers, a moiré pattern is created which gives rise to many surprising new properties. In my talk, I will describe how the atomic, electronic and optical properties of these systems can be described using atomistic techniques ranging from large-scale density-functional theory and tight-binding approaches to many-body techniques, such as the Bethe-Salpeter equation. I will discuss how the multi-valley electronic structure of transition metal dichalcogenide (TMD) monolayers gives rise to highly tunable electronic and optical properties in twisted bi- and trilayer systems and describe how the competition of electron-hole interactions and the moiré potential produces different types of excitons, including large-radius Wannier excitons and unconventional intra-layer charge-transfer excitons. Finally, the anomalous diffusion of excitons in twisted bilayers due to the strong coupling to interlayer shear vibrations (phasons) will be discussed.

Non-reciprocal phase transitions

Peter Littlewood[3,4], R Hanai[1,5], S Liu[3], C Weis[3], M Fruchart[5], V Vitelli[3]
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Session: Non-equlibrium and Quantum Thermodynamics, July 3, 2024, 14:00 - 16:10

Spontaneous synchronization is at the core of many natural phenomena. Your heartbeat is maintained because cells contract in a synchronous wave; some bird species synchronize their motion into flocks; quantum synchronization is responsible for laser action and superconductivity. The transition to synchrony, or between states of different patterns of synchrony, is a dynamical phase transition that has much in common with conventional phase transitions of state – for example solid to liquid, or magnetism – but the striking feature of driven dynamical systems is that the components are "active". Consequently quantum systems with dissipation and decay are described by non-Hermitian Hamiltonians, and active matter can abandon Newton's third law and have non-reciprocal interactions. This substantially changes the character of many-degree-of-freedom dynamical phase transitions between steady states and the critical phenomena in their vicinity, since the critical point is an "exceptional point" where eigenvalues become degenerate and eigenvectors coalesce.

We will illustrate this in several different systems – a Bose-Einstein condensate of polaritons, models of multicomponent active matter such as flocks of birds, generalized Kuramoto models, and others. We argue that there is a systematic theory and generalized phase diagram, and corresponding universality behaviors determined by the symmetry of the models.

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Charge-Imbalanced Polaritons

Prof. Francesca Maria Marchetti[1]
[1] *Universidad Autónoma de Madrid, Spain*

Session: Polaritons, July 2, 2024, 10:30 - 12:40

Microcavity exciton-polaritons, the entangled superposition of an exciton and a cavity photon, offer unique advantages for the design of the intrinsic properties of photons through matter and, conversely, the manipulation of the properties of matter through light. Recent experimental progress has allowed the study of the interplay between strong light-matter coupling and electronic doping, thereby opening the prospect of generating and controlling novel strongly correlated phases between exciton-polaritons and a 2D electron gas. In this presentation, I will explore the occurrence of different phases in charge-imbalanced mixtures of electrons and holes strongly coupled to a cavity mode, including the possibility for an exotic rotationally broken condensed phase. I will present results from our recent studies on the role of temperature in the optical response of doped two-dimensional semiconductors. These findings, in excellent agreement with recent experiments on doped monolayer MoSe2, allow to formally unify two distinct theoretical approaches that have been applied to this system, with the conventional trion picture emerging as a high-temperature and weak-interaction limit of the Fermi polaron theory.

Controlling charge transfer in metastable nanostructures and topological 2D materials

Reinhard Maurer[1]
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Session: Surface Physics/2D Materials, July 3, 2024, 14:00 - 16:00

At hybrid metal-organic interfaces, localized molecular electronic levels couple with a continuum of electrons in the substrate. This can potentially yield charge rearrangements at the interface. This effect is of great relevance during the formation of organic-metallic thin-films, during molecular gas-surface reactions, and when manipulating single molecules at surfaces. The interfacial level alignment is sensitive to dynamic molecular motion, to impurities and defects, and to changes in the electronic structure. By understanding these effects from first principles, we advance our ability to design nanostructures and their properties from the bottom up.
In this talk, I will show how state-of-the-art electronic structure theory, surface spectroscopy simulations and molecular dynamics simulations at surfaces provide insights into static and dynamic charge-transfer at interfaces, which controls structure and measurable electronic and spectroscopic properties of materials. I will cover examples ranging from self-assembled two-dimensional donor-acceptor networks [1], bottom-up design of topological defects in graphene, [2] to single atom and molecule manipulation. [3]

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Ferromagnetic quantum criticality in Fe(Ga1-xGex)3

Prof. Alix Mccollam[1]
[1] *University College Cork, Ireland*

Session: Strongly Correlated, July 3, 2024, 14:00 - 16:10

Magnetic quantum critical points in strongly correlated electron systems promote the emergence of novel phases and properties. Ferromagnetic quantum critical points (FM-QCP) are avoided in most systems, so relatively little is understood about their effect on the wider phase diagram. The 3d-electron system Fe(Ga1−xGex)3 is a candidate to show a FM-QCP, and gives us the opportunity to characterise the associated electronic and magnetic behaviour. FeGa3 is a diamagnetic semiconductor that becomes metallic with a small amount of Ge doping. A weak ferromagnetic moment develops in Fe(Ga1-xGex)3 at a critical doping of xC ~ 0.043-0.05, and grows with further doping up to x ~ 0.1. Close to xC, non-Fermi liquid behaviour has been observed in transport and thermodynamic properties, suggesting a FM-QCP [1]. The nature of the ferromagnetism is still a matter
of debate [2]. I will present transport, including Shubnikov-de Haas oscillations, and magnetic susceptibility measurements of Fe(Ga1-xGex)3, at several dopings in the paramagnetic and ferromagnetic phases. We find
strange metal behaviour at high temperature, extending to the lowest measured temperature only near critical doping, and demonstrating an element of classic quantum critical behaviour in this system [3]. There is no indication that the FM-QCP is avoided. Quantum oscillations show that the Fermi surface changes significantly from the paramagnetic to the ferromagnetic phase, indicating a complicated bandstructure, particularly in the paramagnetic phase, that is not captured by current DFT calculations. In the ferromagnetic phase, magnetic susceptibility suggests the formation of domain walls that become increasingly mobile with increasing Ge content.

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Energy transport and refrigeration with driven quantum dots

Juliette Monsel[1]
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Session: Non-equlibrium and Quantum Thermodynamics, July 3, 2024, 14:00 - 16:10

Thermal transport in quantum dots has been extensively studied in the context of steady-state heat engines, e.g. [1]. However, quantum dots are also relevant for cyclic thermal machines as they can be time-dependently driven, e.g., to pump charge. Understanding the characteristics of energy transport in slowly-driven quantum dots is therefore important. I will present the simple case of a driven single-level quantum dot weakly coupled to two electronic contacts. The dot has an onsite interaction, which can be either repulsive, like the typical Coulomb interaction, or attractive, as realized experimentally, e.g. in [2-4].

In the first part, I will focus on the case of slow driving, allowing for a geometric approach that we combined with a fermionic duality for the evolution operator of the master equation [5], which provides compact and insightful analytic expressions [6]. I will show the concrete effects of strong many-body interaction and the impact of the interaction sign on energy transport. Then, I will explain how to use this device as a heat pump or refrigerator and highlight the crucial role of the interaction sign in the performances of these thermal machines. In the second part, I will present a more traditional 4-stroke thermodynamic cycle to operate the dot as a refrigerator and show the impact of the onsite interaction on the thermal machine performances, from strongly attractive to strongly repulsive, through weak interaction strength [7].

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Antiferroelectric-like behaviour in tetragonal tungsten bronzes

Finlay Morrison[1]
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Session: New Materials 1, July 2, 2024, 10:30 - 12:30

Since its discovery in the 1950s, antiferroelectricity has largely been perceived as an academic curiosity as the electric analogue of antiferromagnetism. However, there has been much recent interest in antiferroelectric materials for high voltage, high power capacitors. After perovskite (ABO3), the tetragonal tungsten bronzes, TTBs, (A12A24B12B28O30) form the largest structure family of ferroelectric oxides. TTBs have much more diverse and complex compositional and structural flexibility than perovskites and recently have been shown to also exhibit antiferroelectric behaviour. Two such examples are the highly non-stoichiometric or “empty” Ba4Ln0.67Nb10O30 and filled K4Ln2Nb10O30 TTB families where Ln = lanthanoid. In both cases antiferroelectric behaviour arises due to a field-induced phase transition, however, detailed structural analysis using synchrotron X-ray, neutron and electron diffraction experiments (including in-situ under applied field) coupled with electrical property measurements show that the underlying structural mechanisms are subtly different in these two materials. I will discuss our recent work on these TTBs, highlighting the key differences in the origin of their antiferroelectric-like behaviour.

A computational hunt for conventional high temperature superconductivity

Prof Chris Pickard[1]
[1] *University of Cambridge, United Kingdom*

Session: Electronic Structure 1, July 3, 2024, 10:30 - 12:40

First principles methods for the prediction of the structure of materials have delivered a powerful tool for generating candidate structures for comparison with experimental analytical methods. Early studies focused on the exotic properties and structures of relatively simple systems, typically the elements and binary compounds. The promise of discovering materials with extreme properties relies on the ability of screen a wide variety of compounds.[1] I will reflect on why ab initio random structure searching (AIRSS) is particularly suited to these challenges, focussing on the dramatic acceleration that ephemeral data derived potentials (EDDPs) afford,[2] and their role in the uncovering of Mg2IrH6 as a feasible ambient pressure high temperature superconductor.[3]

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Synthesis and crystal growth in extreme conditions: Around perovskite and Ruddlesden-Popper Nickelates

Pascal Puphal[1]
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Session: Superconductivity 2, July 3, 2024, 14:00 - 16:10

High Tc superconductivity remains one of the main focuses in condensed matter research, in which, rare-earth nickel oxides have emerged as a new class with potential for unconventional superconducting behavior. Here, two types of structures have drawn particular interest:
The first are nickelates with the infinite-layer crystal structure, such as Nd0.8Sr0.2NiO2, with superconducting transition temperatures up to 20 K.
The second type was found in Ruddlesden-Popper (RP) phase nickelates, such as La3Ni2O7, which under hydrostatic pressure realize a remarkably high Tc of 80 K.
Many details of these systems are not yet fully understood especially as for the first type only thin films show superconductivity up to now. In my talk I will show the challenges of optimal doping perovskite single crystals in high oxygen pressures, and show the advancements we have done in obtaining optimal reduced crystals as well as the effects of intercalation on these single crystals.
Furthermore, I present our findings on La4Ni3O10, La3Ni2O7, where sizable single crystals can be readily grown using the optical floating zone. Here, we recently observed that these crystals exhibit multiple crystallographic phases and a pronounced sensitivity to oxygen stoichiometry, affecting their physical properties and fascinating pressure dependence as will be highlighted in the talk. Finally, I will present a sub-family of nickelates and discuss their relevance to the existing RP.

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Probing Quantum Processes in Condensed Matter with Extreme Spatiotemporal Precision

Prof Akshay Rao[1]
[1] *University of Cambridge, United Kingdom*

Session: Hybrid Organic/Inorganic, July 3, 2024, 10:30 - 12:40

Time-resolved spectroscopy has for a number of decades provided rich insights into the non-equilibrium physics of a range of condensed matter systems, such as semiconductors, plasmonic, polaritonic and strongly correlated materials. Here we will present first results from a new spectroscopic and microscopic methodology that pushes the limits of what can be achieved in terms of time-resolution, spatial precision, and energy ranges. Via directly reading out the electric field of ultrafast light pulses, we achieve sub-cycle temporal resolution, below 100 attoseconds, combined with spatial precision below 100nm, across a large energy range spanning the UV to SWIR. We will explore the possible uses of this new platform for probe fundamental processes in condensed and quntum matter.

The magic angle of Sr2RuO4: Optimising correlation-driven superconductivity

Dr Luke Rhodes[1]
[1] *University of St Andrews, United Kingdom*

Session: Tuning many-body interactions, July 4, 2024, 14:00 - 16:05

A fundamental understanding of unconventional superconductivity is crucial for engineering materials with specific order parameters or elevated superconducting transition temperatures (Tc). However, for many superconducting materials, such as Sr2RuO4, the pairing mechanism and symmetry of the superconducting order parameter remain unclear.

Here, I will discuss the theoretical progress we've made to address the mysteries surrounding superconductivity in Sr2RuO4 [1]. In particular focusing on understanding how small structural distortions should influence the superconducting transition temperature and order parameter assuming an electron-correlation driven pairing mechanism. I'll discuss how the conventionally used Random Phase approximation (RPA) is insufficient to describe the known experimental data and that competing fluctuation channels, as captured in functional renormalisation group theory (FRG), are essential to reproduce the known increase in Tc under uniaxial strain and the suppression of Tc upon large rotations of the RuO6 octahedra, as observed at the surface of Sr2RuO4. Furthermore, within this framework we find an even greater enhancement of Tc for small rotations of the RuO6 octahedra, with a predicted maximum over twice as large as the current maximum Tc found under uniaxial strain.

Finally, by incorporating the results obtained from either the RPA and FRG techniques into a simple, yet realistic, superconducting Hamiltonian, I'll present a method that can provide new direct tests for distinguishing the superconducting order parameter in unconventional superconducting materials from experimental probes.

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Time-Resolved Photoelectron Diffraction: Mapping Atomic Motion in Phonon Oscillations

Charlotte Sanders[1], D Curcio[2], K Volckaert[2], D Kutnyakhov[3], S.Y. Agustsson[2,4], K Bühlmann[5], F Pressacco[3], M Heber[3], S Dziarzhytski[3], S Acremann[5], J Demsar[4], W Wurth[3,6], PH Hofmann[2]

[1]STFC Central Laser Facility, United Kingdom, [2]Interdisciplinary Nanoscience Center (iNANO), , Denmark, [3]Deutsches Elektronen-Synchrotron DESY, Germany, [4]Johannes Gutenberg-Universität, Germany, [5]Laboratory for Solid State Physics, Switzerland, [6]Hamburg University, Germany

Session: Ultrafast/2D, July 5, 2024, 10:30 - 12:40

X-ray photoelectron diffraction (XPD) is a technique that is based on the tools of X-ray photoelectron spectroscopy (XPS). It combines chemical sensitivity with the power to elucidate local geometric order at surfaces. Free-electron lasers (FELs) can deliver ultra-short X-ray pulses in an energy range suitable for XPD study. The fact that FEL pulse trains can be synchronized with those of secondary, lower-photon-energy laser sources means that XPD can potentially be adapted to pump-probe, time-resolved studies. This would expand the technique's scope: for example, to permit visualization of complex phonon modes and surface catalytic processes. We have now used pump-probe XPD at the PG2 beamline of the FLASH free-electron laser (FEL) to demonstrate time-resolved XPD measurements of the "simple" model system Bi2Se3 [5]. Key to the success of this experiment is the HEXTOF experimental station, which is based on a time-of-flight (ToF) momentum microscope (MM). We pump the A_1g^1 phonon mode with a tabletop laser system, and demonstrate that we can observe oscillations in the interlayer spacings near the surface of the crystal.

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Exploring new superfluid phenomena in polariton condensates

Daniele Sanvitto
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Session: Polaritons, July 2, 2024, 10:30 - 12:40

Polaritons are unique quasiparticles resulting from the coupling of excitons with confined photons in semiconductors. Their hybrid light-matter nature has facilitated the study of various fundamental phenomena and the proposal of numerous technologically relevant applications, offering advantages such as low energy consumption, dissipation-less operation, and high clock frequencies. [1] Moreover, polaritons exhibit captivating macroscopic quantum phenomena, including superfluidity, quantized circulation, and parametric effects, to name a few.

In this work, we first explore the potential observation of supersolid formation in a polariton condensate. By utilizing patterned waveguides to fold propagating polariton modes within the light cone, we induce the creation of topologically protected states where condensation occurs at very low thresholds. [2-4] Through the spontaneous parametric scattering into higher modes within the waveguide, we observe a modulation atop the condensate, suggesting the emergence of a supersolid phase.

In a second part of this work, we will show the realization of a weak link in a tilted polariton ring condensate with an induced net current flow within the ring. Our investigation reveals the realization of Josephson currents in a ring geometry, with the tunneling current under the barrier showing a sinusoidal relationship–despite the circulation imposed on the bosonic fluid–characteristic of Josephson physics. [5]

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Altermagnetism: from spintronics to unconventional magnetic phases

Libor Smejkal[1]
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Session: Magnetism 3, July 5, 2024, 10:30 - 12:30

The search for unconventional quantum phases that break the symmetries of the crystal lattice has been a focus in physics since the early days of quantum theory, driven by both fundamental interest and potential applications. Prominent examples include cuprate superconductors, which are known for their unconventional d-wave Cooper pairing, and dissipationless transport.

In this presentation, we will discuss our recent discovery[1] of an unconventional magnetic phase motivated by our earlier predictions and observations of unconventional spintronics effects [2,3,4]. This unconventional altermagnetic phase (see Figure), unlike common ferromagnetism and antiferromagnetism, breaks the symmetries of the crystal lattice, and features d, g, or i-partial wave characteristics simultaneously in its spin and electronic structure[1]. D-wave altermagnetism thus represents magnetic analogue of d-wave superconductivity.

We identified altermagnetism by employing and developing a symmetry framework that considers paired transformations involving electron spin and the crystal lattice. This framework is emerging as a new paradigm in the study of magnetic crystals. We will demonstrate its usefulness by discussing (i) the altermagnetic band structure of the semiconductor MnTe, which we recently experimentally observed through collaborative work using photoemission spectroscopy[5], and (ii) our identification of more than 240 realistic altermagnetic candidates.

Additionally, we will explore the rapid expansion of altermagnetic concepts to many fields with focus on ultrafast spintronics memories[6], dissipationless transport [2-4] and two-dimensional band topology [7]. Finally, we will outline the latest developments in the field, including our theoretical identification of p-wave magnetism, an analog of superfluid helium-3, and we will propose transport experiments which can be used for its detection[8].

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Computational materials modelling of rare earth - transition metal magnets

Prof. Julie Staunton[1]
[1] *University of Warwick, United Kingdom*

Session: Magnetism 1, July 2, 2024, 10:30 - 12:40

In this talk first-principles calculations for a quantitative model of rare earth - transition metal magnets, inspired by the 'standard model', will be described for the extensively used strong magnet, Nd2Fe14B. A rich and complex behaviour originating from the Fe atoms, is revealed which tends to be missed out currently from larger-scale simulations (1). Real magnets always contain defects, and these are understood to adversely affect the coercivity, one of the most sought-after properties of commercial magnets. Current state-of- the-art models either assume pristine materials or treat defects heuristically, which limits their predictive power. This talk will introduce a simple but accurate analytical model of defects (2) with parameters determined from our first-principles calculations, which is suitable for deployment in large-scale atomistic spin dynamics calculations and statistical analyses. It will be shown how point defects, in the form of Ti atom substitutions, dramatically modify the magnetocrystalline anisotropy of the archetypal "rare earth-lean" magnet SmFe11Ti.

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A new 2D platform for quantum technology: A quantum coherent spin in hexagonal boron nitride that operates at ambient conditions

Hannah Stern[1]
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Session: Materials for Quantum Technologies 2, July 4, 2024, 10:30 - 12:30

Solid-state spin-photon interfaces that combine single-photon generation and long-lived spin coherence with scalable device integration, ideally at ambient conditions, hold great promise for the implementation of quantum networks and sensors [1]. Despite rapid progress reported across several candidate systems, those possessing quantum coherent single spins at room temperature remain extremely rare. In this talk I will show quantum coherent control under ambient conditions of a single-photon emitting defect spin in a layered van der Waals material, hexagonal boron nitride [2]. We identify that the carbon-related defect has a spin-triplet electronic ground-state manifold and demonstrate that the spin coherence is governed predominantly by coupling to only a few proximal nuclei and is prolonged by decoupling protocols. These results serve to introduce a new platform to realise a room-temperature spin qubit coupled to a multi-qubit quantum register or quantum sensor with nanoscale sample proximity.

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Charge Carrier Recombination and Transport in Halide Perovskite Semiconductors

Professor Sam Stranks[1]
[1] *University of Cambridge, United Kingdom*

Session: Hybrid Organic/Inorganic, July 3, 2024, 10:30 - 12:40

Halide perovskites are generating enormous excitement for next-generation optoelectronic devices including photovoltaics, light-emitting diodes (LEDs) and detectors. Here, I will outline recent work in our group towards the development and understanding of halide perovskite semiconductors. I will cover topics including recombination and charge transport on different length scales in 3D absorbers as well as 2D and 2D/3D thin films with either passive or electro-active organic linkers. Such developments are leading to new photophysical understanding, further increased performance and new device platforms.

Topological Surface State in a Spin-triplet Superconductor

Dr Shuqiu Wang[1]
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Session: Superconductivity 3, July 4, 2024, 10:30 - 12:40

The interplay of superconductivity and topology stands at the frontier of moden quantum matter physics. Intrinsic topological superconductivity is important because its electronic properties are topologically protected and robust against local perturbations. Although topological superconductivity appears probable in UTe2, its superconductive order parameter Δ_k has not yet been established. If spin-triplet, it should have odd parity so that Δ_(-k)=-Δ_k and, in addition, may break time-reversal symmetry. A distinctive identifier of such nodal spin-triplet superconductors is the appearance of an Andreev bound state (ABS) on surfaces parallel to a nodal axis, in the form of a topological surface band (TSB). Moreover, theory shows that specific TSB characteristics observable in tunneling to an s-wave superconductor distinguish between chiral and non-chiral Δ_k. To search for such phenomena in UTe2, we employ s-wave superconductive scan-tip imaging [1] and discover a distinct TSB signature, an intense zero-energy Andreev conductance maximum at the (0-11) crystal termination. Its imaging yields quasiparticle scattering interference evidence for two Δ_k nodes aligned with the crystal a-axis. Most critically, development of the zero-energy Andreev conductance peak into two finite-energy particle-hole symmetric conductance maxima as the tunnel barrier is reduced, signifies that UTe2 superconductivity is non-chiral. Overall, this combination of a zero-energy Andreev conductance maximum at the UTe2 (0-11) surface, internodal scattering along the a-axis, and splitting of Andreev conductance maximum due to s-wave proximity, categorizes the superconductive Δ_k of UTe2 as the odd-parity non-chiral topological state [2].

[1] Nature 618, 921 (2023).
[2] Gu, Wang, Carroll et al., Science in Review (2024).

Adding spin control to a quantum dot-based single-photon source

Professor Richard Warburton
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Session: Materials for Quantum Technologies 3, July 4, 2024, 14:00 - 16:00

We have recently reported a single-photon source using a single semiconductor quantum dot in an open microcavity [N. Tomm et al, Nature Nanotechnology 16, 399 (2021)]. The end-to-end efficiency, the probability of creating a single photon at the end facet of the output fibre, is above 50%; the coherence of the photons as judged by the two-photon interference visibility, is high, 98%. In order to create more complex photonic states, entangled photon-pairs and cluster states, it is necessary to add the spin degree of freedom. The Achilles heel of the quantum-dot system is the poor spin coherence (small T2*) on account of the spin noise of the host nuclei. Here, a single hole is added to the quantum dot, and its spin is rotated around the Bloch sphere by a Raman process. We report ultrahigh Rabi frequencies, up to 1 GHz, and an almost-complete suppression of the nuclear-spin noise by laser-cooling the nuclei. The hole-spin T2* (500 ns) becomes much larger than both the Purcell-enhanced radiative recombination time, 50 ps, and the time required to complete a spin rotation, potentially enabling many spin-photon pairs to be created before the spin loses its coherence.

An alternative bulk-boundary correspondence: ferromagnetism at the surfaces of antiferromagnets

Sophie Weber[1]
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Session: Electronic Structure 2, July 4, 2024, 10:30 - 12:30

Theoretical arguments [1,2] and experimental measurements [3-6] have definitively shown that antiferromagnets (AFMs) with particular bulk symmetries can possess a nonzero magnetic dipole moment per unit area or ``surface magnetization" on certain surface facets. Such surface magnetization underlies intriguing physical phenomena like interfacial magnetic coupling, and can be used as a readout method of antiferromagnetic domains. Here, I present our recent theoretical work [7] where we develop a universal classification and theory of AFM surface magnetization based on properties of the material bulk. Specifically, we show a one-to-one mapping caused by symmetry lowering due to a creation of a surface, and symmetry lowering due to an applied electric field in the bulk. This means that the presence or absence of magnetization on any surface termination and bulk AFM of interest can be determined by the allowed magnetoelectric responses, at linear and higher orders, or equivalently, by the ordering of magnetic multipoles in the bulk unit cell. I will also show density functional calculations, as well as magnetotransport measurements by collaborators [8], which support our symmetry-based predictions that nominally compensated surfaces in magnetoelectric Cr2O3 and altermagnetic FeF2 develop a finite magnetization density. Finally, I will briefly describe a few ongoing efforts involving both potential use cases, as well as practical challenges, for the exploitation of AFM surface magnetization.

[1] A. F. Andreev, JETP Lett. 63, 756 (1996)
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[4] N. Wu et al., Phys. Rev. Lett. 106, 087202 (2011)
[5] P. Appel et al., Nano Lett. 19, 1682 (2019)
[6] M. S. Wörnle et al., Phys. Rev. B 103, 094426 (2021)
[7] S. F. Weber, A. Urru et al., Phys. Rev. X 14, 021033 (2024)
[8] O. V. Pylypovskyi, S. F. Weber et al., Phys. Rev. Lett. 132, 226702 (2024)

Chiral-induced Unidirectional Spin-to-charge conversion

Angela Wittmann[1]
[1] *University of Mainz, Germany*

Session: Ultrafast/2D, July 5, 2024, 10:30 - 12:40

The chiral-induced spin selectivity (CISS) effect has recently gained significant attention in the field of spintronics. The remarkably high polarization efficiency of chiral molecules via the CISS effect paves the path toward novel, sustainable hybrid chiral molecule magnetic applications. While research has predominantly focused on transport properties so far, in our work, we explore spintronic phenomena at hybrid chiral molecule magnetic interfaces to elucidate the underlying mechanisms of the chiral-induced spin selectivity effect. For this, we investigate the interfacial spin-orbit coupling in chiral molecule/metal thin film heterostructures by probing the chirality and spin-dependent spin-to-charge conversion. Our findings validate the central role of spin angular momentum for the CISS effect, paving the path toward the functionalization of hybrid molecule-metal interfaces via chirality.

The pressure-induced CDW transition in CeTe3 probed by time-resolved spectroscopy

Dr Priyanka Yogi[1], C.V. Kotyada[1], J. Tauch[2], H. Schäfer[2], M. Obergfell[2], A. Pashkin[3], Professor Jure Demsar[1]

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Session: Strongly Correlated, July 3, 2024, 14:00 - 16:10

We use time-resolved optical spectroscopy to study pressure-induced charge-density-wave (CDW) phase transition in a prototype CDW system CeTe3 (Tc ~540 K at ambient pressure [1]). Photoinduced reflectivity traces at 300 K and ambient pressure reveal the presence of numerous oscillatory modes with frequencies between 1.2 and 4 THz. The modes display either softening or hardening as a function of pressure, yet all disappear above ~ 5 GPa. Moreover, these modes are quenched above critical photoexcitation density. We compare the pressure and excitation density dependent mode parameters with the available temperature, chemical- and hydrostatic-pressure dependent Raman data on RTe3 series [1]. We show that all modes are CDW amplitude modes, a result of linear coupling between the electronic order and normal-state phonons at the CDW wavevector [2]. Thus, the studies reveal a pressure-induced transition into the metallic state taking place in CeTe3 at the critical pressure of ~ 5 GPa at 300 K.

[1] K. Yumigeta, et al., APL Mater. 10, 111112 (2022); M. Lavagnini, et al., PRB 78, 201101 (R) (2008).
[2] K. Warawa, et al., PRB 108, 045147 (2023), H. Schäfer, et al., PRL 105, 066402 (2010).

Materials for Quantum Technologies - Materials Horizon Scanning Session

Nitrogen Vacancy Centres, a Versatile Testbed for Quantum Sensing and Simulations

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Session: Materials for Quantum Technologies - Materials Horizon Scanning, July 3, 2024, 10:30 - 12:40

In recent years, solid-state systems have been at the forefront of quantum technology research. Among these, the Nitrogen vacancy center (NV) in diamond stands out as a remarkable optically active defect. Its unique properties, including long coherence time, ease of initialization and readout, and coupling to nearby individual nuclear spins, make it an ideal platform for quantum sensing and simulations. In our laboratory, we utilize NVs implanted at varying depths and with different nitrogen concentrations. Our research focuses on nano-scale NMR using shallow implanted NVs and manipulation of individual nuclear spin coupled to the NVs, in bulk NV samples, by employing XY8-n, PulsePol and adiabatic PulsePol sequences.
During this presentation, I will present our recent experiments on the implementation of NV-mediated indirect nuclear spin manipulation techniques. We achieve efficient nuclear spin polarization and arbitrary nuclear spin state preparation using a combination of XY-n [1], PulsePol [2], and adiabatic pulse-sequences [3] in bulk diamond NV samples and compare the efficiency of different techniques. With these capabilities we aim to establish this coupled NVs-nuclear spins system as a reliable and robust room temperature testbed for quantum simulations, allowing us to explore quantum thermodynamics [4] and driven many-body systems [5], towards investigation of quantum devices.

References
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[3] Whaites et al., PRR. 4, 013214 (2022)
[4] Pal et al., Phys. Rev. A 100, 042119 (2019)
[5] Pal et al., Phys. Rev. Lett. 120, 180602 (2018)

Towards Rydberg mediated quantum applications in cuprous oxide

Dr Sai Kiran Rajendran[1], Anindya Paul[1,2], Konstantinos Orfanakis[1], David Ziemkiewicz[3], Thomas Volz[2], Hamid Ohadi

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Session: Materials for Quantum Technologies - Materials Horizon Scanning, July 3, 2024, 10:30 - 12:40

Rydberg excitons in cuprous oxide have attracted immense interest since the observation of high principal quantum number (n) excitons as high as n=25. The non-linearity of these excitons to external fields and their Bohr radii scale exponentially leading to giant micron sized excitons demonstrating Rydberg blockade effects.

We study the novel properties of these Rydberg excitons using cryogenic spectroscopy. We employ two different approaches in order to tune the properties of these excitons. The first approach is to couple Rydberg excitons in a bulk crystal to confined photons in a microcavity. We demonstrate strong exciton-photon coupling of Rydberg excitons as high as n=6 and reveal what limits the coupling of high n Rydberg states.[1] In the second approach, we spatially confine Rydberg excitons to nano-dimensions. In nanoparticles of particular size distribution, we observe changes to the exciton oscillator strength and spectral broadening as a result of quantum confinement.[2] In etched out individual micropillars, we observe size dependent optical tuning of Rydberg energy levels due to thermal effects.[3]

These studies are of immense interest towards the exploitation of excitons for solid state applications using Rydberg mediated single particle quantum non-linearity.

References:
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[2] Quantum confined Rydberg excitons in Cu2O nanoparticles. Phys. Rev. B 103, 245426 (2021)
[3] Local tuning of Rydberg exciton energies in nanofabricated Cu2O pillars. Communications Materials 5, 43, (2024)

Quantized transport in one-dimensional nanowire-graphene spin injectors

Daniel Burrow[1], Jesus C. Toscano-Figueroa[1], Victor H. Guarochico-Moreira[1], Khalid Omari[1], Irina V. Grigorieva[1], Thomas Thomson[1], **Ivan Vera Marun**[1]
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Session: Materials for Quantum Technologies - Materials Horizon Scanning, July 3, 2024, 10:30 - 12:40

The potential of 2D (van der Waals) materials for spintronics has been recognized since graphene was first isolated [1]. However, realizing the early promise of low-power spintronics for next generation classical and quantum computation has proved challenging, in part due to the nature of the interface between a ferromagnetic metal needed to spin polarize injected electrons into the graphene transport layer and spin transport in the graphene layer. Encapsulating graphene in h-BN provides a platform that allows mobilities in excess of 100 000 cm2 V−1 s−1 and spin diffusion lengths approaching 20 μm [2].

In this presentation we report recent advances in high-mobility spintronics by building on our developed architecture [2, 3] which has shown spin-polarized contacts at the 1D edge of h-BN encapsulated graphene. We demonstrate the detection of quantized conductance in the absence of an applied magnetic field, and quantum Hall transport, at one-dimensional spin injecting contacts between magnetic nanowires and record high-mobility graphene spin transistors. The nanowires define an effective quantum point contact at the graphene edge, even in the absence of any constriction in the graphene itself. The demonstration of ballistic spin injection is a milestone in the development of 2D ballistic spintronics.

[1] E.W. Hill et al., IEEE Trans. Magn., 42, 2694 (2006)
[2] V.H. Guarochico-Moreira et al., Nano Letters, 22, 935–941 (2022)
[3] C.R. Anderson et al., Sci Rep 13, 10343 (2023)

Contributed Talks

Incommensurately modulated charge density wave structure of BaAl4 type compounds

Dr. Harshit Agarwal[1], Mr. Surya Rohith Kotla[1], Dr. Sitaram Ramakrishnan[2], Mr. Claudio Eisele[1], Dr. Leila Noohinejad[3], Dr. Martin Tolkiehn[3], Dr. Carsten Paulmann[3], Dr. Biplab Bag[4], Mr. Bishal Baran Maity[5], Dr. Shovan Dan[5], Prof. Dr. Arumugam Thamizhavel[5], Prof. Dr. Srinivasan Ramakrishnan[2], Prof. Dr. Sander van Smaalen[1]

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Session: Strongly Correlated, July 3, 2024, 14:00 - 16:10

In recent years, intermetallic compounds with the BaAl4 structure type have attracted attention for their properties as topological quantum materials. The compounds R(Al1-xGax)4 (where R= Eu, Sr) have a tetragonal crystal structure with space group I4/mmm at room temperature [1]. The temperature dependence of electrical resistivity of these compounds suggests the formation of a charge density wave (CDW) in EuAl4 at TCDW = 145 K [1], in SrAl4 at TCDW = 243 K [2], and in EuGa2Al2 at TCDW = 51 K [1]. Crystal structures of the incommensurately modulated CDW phases have been described by the superspace theory [3]. Single-crystal X-ray diffraction (SXRD) reveals an incommensurately modulated orthorhombic CDW phase in EuAl4, with modulation wave vector q = (0, 0, 0.174) at 20 K, and superspace group Fmmm(00g)s00 [4]. Second-order satellite reflections in the SXRD data of SrAl4 point towards a loss of inversion symmetry. SrAl4 has a CDW state with modulation vector q = (0, 0, 0.1116) at 200 K and the noncentrosymmetric superspace group F222(00g)00s [5]. We will present the structure analysis of incommensurately modulated CDW crystal structure in EuAl2Ga2 and its comparison to the CDW structures of EuAl4 and SrAl4 using the superspace group approach.

Reference:
1. M. Stavinoha et al, Phys. Rev. B 97, 195146 (2018)
2. Nakamura et al., J. Alloys Compd. 654, 290 (2016)
3. S. van Smaalen, Incommensurate Crystallography, Oxford University Press (2007)
4. S. Ramakrishnan et al., IUCrJ, 9, 378, (2022)
5. S. Ramakrishnan et al., (2023) arXiv: 2309.08959

Probing the magnetism of CrTe2 using quasiparticle interference

Olivia Armitage[1], Naina Kushwaha[1], Akhil Rajan[1], Phil D. C. King[1], Peter Wahl[1,2]
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Session: 2D Materials 1, July 3, 2024, 10:30 - 12:40

Two-dimensional magnetic materials have potential applications in spintronic devices, as well as being important in expanding the range of tuneable properties of van der Waals heterostructures. However, the electronic and magnetic properties of these materials can be difficult to determine, as many techniques measure over a large area, resulting in an average over different magnetic domains. To probe the unaveraged electronic structure, samples must be measured on the scale of tens of nanometres. Here, we use scanning tunnelling microscopy (STM) to investigate the local electronic and magnetic properties of monolayer samples of the magnetic material CrTe2. By comparing experimental and simulated quasiparticle interference patterns and relating these to possible scattering processes identified from the density functional theory-calculated band structure, we are able to identify the ground magnetic state of the sample. We also present angle-resolved photoemission spectroscopy measurements and compare these to the STM data and theoretical band structure calculations.

Bridging the visible and mid-IR with exciton plasmon-polaritons for mid-IR detection

Dr. Rakesh Arul[1], Fiona Bell[1], Lille Borresen[1], Piper Fowler-Wright[2], Zhongzheng Yu[1], Akshay Rao[1], Jonathan Keeling[2], Jeremy Baumberg[1]
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Session: Polaritons, July 2, 2024, 10:30 - 12:30

The infrared (IR) spectrum of molecules contains rich structural information, enabling disease diagnosis, greenhouse gas monitoring, and the stunning images of exoplanets. Despite such promise, IR detection remains far from democratized due to the costs and limited practical utility of existing technologies. To circumvent this, we take advantage of efficient silicon sensors in the visible to help detect IR, which requires converting IR to detectable visible light. While theoretically proposed by Bloembergen in 1959, realising this conversion has proven challenging due to wavelength mismatch and poor efficiency.

We found that layers of gold nanoparticles, assembled with precise spacing using a dye molecule, possess dual IR and visible plasmon-polaritons, enhancing the local optical field by many orders-of-magnitude. These layers allow conversion of mid-IR light into visible light and the detection down to single molecules. This opens a new area of studying mid-IR fluctuation spectroscopy. Additionally, by placing lanthanide nanocrystals between these layers of gold nanoparticles, mid-IR light can be directly converted into visible light, enabling practical detectors.

Using ultrafast spectroscopy, we measure the vibrational coherence lifetimes of molecules within plasmonic nanogaps, observing a new vibrational cascade mechanism in the formation of collective excitonic states. Measurements of spatio-temporally resolved g(1) correlations of visible light emission reveals the formation of a new exciton plasmon-polariton condensate, amplifying the mid-IR upconversion process.

These observations point to a new kind of room-temperature condensate, only present in plasmonic nanostructures with strong light confinement. This launches new ways of detecting mid-IR light and understanding fundamental light-matter interactions.

Magnon-Magnon Coupling in a Pinned Synthetic Antiferromagnet

Dirk Backes[1]
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Session: Magnetism 3, July 4, 2024, 10:30 - 12:30

Magnon-magnon coupling garnered considerable interest lately because of the novel spin-wave states that can be observed, coherently overlapping over a large volume. A synthetic antiferromagnet (SAF) is the ideal model system to study such coupling effects, as it can harbour both optical and acoustic magnon modes. Under certain circumstances, these modes can mix or hybridise into magnon bands exhibiting a band gap, a measure for the coupling strength.

We demonstrate magnon-magnon coupling in a SAF using a home-built, VNA-based ferromagnetic resonance spectroscopy setup. Exciting both modes at the same time can be tedious, posing special requirements at the waveguide or cavity design [1]. Our method is compatible with any given FMR setup and relies on pinning the SAF to an antiferromagnet. We show that, even in the weak pinning case, a magnon band gap of several GHz can be produced. This band gap is independent of the sample orientation with respect to the waveguide, requires no cooling and just a moderate magnetic field of <0.5T.

Highly coherent magnon-magnon coupling states have the potential to be integrated and entangled with quantum platforms including superconducting qubits, nitrogen-vacancy centres, cavity photons, and phonons for coherent information transfer and collaborative information processing [2]. Our work thus paths the way towards applications in quantum computing, quantum memories and high-precision measurements.

[1] A. Sud et al., Phys. Rev. B 102, 100403(R) (2020)
[2] D. D. Awschalom et al., IEEE Trans. Quantum Eng. 2, 5500836 (2021)

Synthesize of Iron selenide layers via salt-assisted chemical vapor deposition

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[1]*School of Chemical and Physical Sciences, Keele University, United Kingdom*

Session: New Materials 1, July 2, 2024, 10:30 - 12:30

Iron selenide compounds (FexSey) are an emerging class of materials known for their remarkable superconducting, catalytic and magnetic properties. It has been established that single-layer tetragonal iron selenide (FeSe) is an excellent superconductor at a critical temperature of ~55 K. While other stoichiometries can have drastically different properties, for example, Fe3Se4 presents metallic features similar to that of other transition metal chalcogenides (TMCs). Other stable stoichiometric compounds exhibit similar properties, for instance, FeSe2 and therefore it is clear that Iron selenides have untapped potential for quantum technologies. In this work, we present the epitaxial growth of a range of 2D iron selenide compounds, FexSey on silicon dioxide (SiO2) substrate using a salt-assisted chemical vapour deposition (CVD) method. The iron and selenium ratio can be finely tuned by the weight ratio of precursors selenium and Iron oxide (FeO) powders, and the growth promotor ammonium chloride salt. Furthermore, allowing the growth of various layer thicknesses with triangle and hexagonal morphologies which have the potential to be scaled up to wafer-scale coverage. The as-grown structures were characterized using X-ray diffraction (XRD), Raman and Energy dispersive X-ray (EDX) techniques, showing clear stochiometric control and chemical stability under ambient conditions. These characterization techniques allow the opportunity to explore the role of the growth-promoting ammonium chloride salt in the synthesis process and how this influences the formation of iron selenides or Iron oxide. The successful growth of 2D iron selenide with different stoichiometry and morphologies offers the prospect of applications in quantum technology.

Determination of the superconducting order parameter of Sr2RuO4 by use of phase-referenced Bogoliubov quasi-particle interference.

Rebecca Bisset[1], Luke C. Rhodes[1], Jonas B. Profe[2,3], Matteo Dürrnagel[4,5], Carolina A. Marques[6], Tilman Schwemmer[4], Dante M. Kennes[3,7], Ronny Thomale[4], Chris Hooley[8], Peter Wahl[1,9]

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Session: Superconductivity 3, July 4, 2024, 10:30 - 12:40

The unconventional superconductivity observed in Sr2RuO4 has long captivated the scientific community with much discussion around the superconducting order parameter, yet no consensus has been reached. Phase-referenced Bogoliubov quasiparticle interference (BQPI) presents a novel approach to this issue, but both BQPI and the superconductive state are strongly sensitive to the surface, defect concentrations, and other experimental parameters - making measurement difficult.

Here, we discuss a multifaceted approach to the theoretical prediction and simulation of phase-referenced BQPI as a tool to resolve the debate about the superconducting order parameter. We have combined continuum tight binding calculations with theoretical modelling of the superconducting order parameter to carry out a detailed study of the impact of different superconducting order parameters on the BQPI signal, incorporating the role of surface effects. Subsequently, we extrapolate BQPI features which could be searched for experimentally using data which matches closely with previous experiment. Our method advances understanding of this unconventional superconductor, providing a roadmap for both interpreting future experimental observations and refining theoretical models in this field.

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

Dr Deepnarayan Biswas[1], Dr Matthias Schmitt[2], Dr. Jieyi Liu[1], Dr. Olena Tkach[3], Dr. Olena Fedchenko[3], Prof. Hans-Joachim Elmers[3], Prof. Ralph Claessen[2], Prof. Gerd Schönhense[3], Dr. Tien-Lin Lee[1]
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Session: Ultrafast/2D, July 5, 2024, 10:30 - 12:40

Angle-resolved photoelectron spectroscopy (ARPES) experiments are typically performed with excitation energies below ~100 eV to take advantage of the higher photoionisation cross-sections and better energy and (in-plane) momentum resolutions. However, the very short electron mean free paths at low energies severely limit the bulk sensitivity. It is therefore desirable to extend ARPES to the soft x-ray (SX) range, which opens the possibility to probe unconventional electronic structures at buried interfaces [1], study 3D electronic systems [2], etc.

We are currently commissioning a SX-ARPES end-station at Beamline I09 [3] at DLS, equipped with a state-of-the-art momentum microscope (MM). MMs preserve the momentum view and resolution independent of the excitation energy [4], which is advantageous for ARPES performed at high energies. In addition, MMs allow selective studies of micron/sub-micron sample areas using field apertures. Our MM is uniquely designed to use a single hemispherical analyser followed by a time-of-flight section equipped with a fast delay-line detector as a combined energy filter, resulting in highly efficient data acquisition [5]. Here, I will discuss the current progress and the potential applications of this new facility for quantum materials research.

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Evaluation of the exchange properties of transition metal phthalocyanines using broken symmetry density functional theory

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Session: Surface Physics, July 5, 2024, 10:30 - 12:30

Due to their chemical and thermal stability as well as the variation observed in their magnetic moments, the family of transition metal phthalocyanines (TMPcs) has been studied quite extensively within the context of spintronic applications. Their crystallisation into ordered chains offers an opportunity to fabricate low dimensional, magnetic materials. However, a prerequisite for successful implementation into commercially viable technological devices is magnetisation at, or exceeding, room temperature and, as of yet, no candidates within this class of materials show such ordering. Despite this, alpha-phase cobalt (II) phthalocyanine (α-CoPc) has been reported to exhibit exceptionally strong magnetic coupling with respect to other first-row TMPcs. The underlying reason for this is theorised to originate in its respective electronic configuration. By mapping the features of the system to a simple model Hamiltonian, the dynamics of the mechanism may be parametrised and predictions of how the coupling strength will change with modifications to both chemical structure and geometry can be made. Broken-symmetry density functional theory calculations are used to explicitly evaluate the exchange strength and directed modifications to the system are shown to significantly increase the coupling within the materials.

Investigating the influence of screening on the unconventional charge density wave in monolayer TiSe2

Sebastian Buchberger[1,2], Dr. Philip A. E. Murgatroyd[1], Dr. Brendan Edwards[1], Dr. Akhil Rajan[1], Prof. Phil D. C. King[1]

[1]*University Of St Andrews, United Kingdom,* [2]*Max Planck Institute for Chemical Physics of Solids, Germany*

Session: Ultrafast/2D, July 5, 2024, 10:30 - 12:40

$TiSe_2$ is a layered transition metal dichalcogenide, and it is well established that it exhibits an unconventional charge density wave (CDW) below a critical temperature of ~200K. However, the microscopic mechanism underlying this reconstructed ground state remains controversial [1,2,3]. In its normal state, $TiSe_2$ exhibits a narrow indirect bandgap. Based on this electronic structure, the system was suggested to be an excitonic insulator, an exotic state in which the energy gain from the formation of excitons drives the CDW transition. However, since the electronic reconstruction is accompanied by a periodic lattice distortion, it was also argued that a less exotic structural mechanism may be responsible for the CDW.

Thinning the material down to monolayer thickness provides new opportunities for testing these contradictory hypotheses. Assuming an excitonic mechanism, the strongest possible CDW should occur in a minimally screened environment. To investigate this, we have developed the synthesis of $TiSe_2$ monolayers in epitaxial heterostrucutres with hexagonal boron nitride (hBN), the gold standard dielectric in the class of 2D materials. With a 6eV bandgap, conventional electronic structure measurements using angle resolved photoelectron spectroscopy (ARPES) are impossible on this system. However, by thinning the substrate down to few 10 nanometres, we obtain high-quality μ-ARPES data on this $TiSe_2$/hBN heterostructure. I will present the resulting temperature evolution of the CDW state in this system, and compare it to the reference system $TiSe_2$/graphite to test the long-standing excitonic insulator claims in this material family.

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[3]PRB 103, 205108 (2021)

Electron quantum optics with superconducting devices

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Session: Materials for Quantum Technologies 2, July 4, 2024, 10:30 - 12:30

Electron quantum optics explores coherent single-electron charge pulse propagation in electronic nanoscale circuits akin to table-top photon setups. While past experiments focused on normal-state conductors, incorporating superconductors holds promise for exploiting the electron-hole degree of freedom in quantum sensing applications and quantum information processing. We propose and analyze a tunable mechanism for converting single-electron pulses into holes through Andreev processes on a superconductor [1]. We develop a Floquet-Nambu scattering formalism to demonstrate the dynamic conversion of charge pulses and the controllable generation of coherent electron-hole superpositions through interferometric magnetic flux control. A Wigner function representation also allows us to visualize the response function of the interface both in the time and in the frequency domain [2]. Our discussion covers optimal conditions in realistic scenarios, affirming the feasibility of our proposal with current technology.

[1] P. Burset, B. Roussel, M. Moskalets, C. Flindt, arXiv:2312.13145
[2] B. Roussel, P. Burset, C. Flindt, arXiv:2312.13829

Intercavity polariton slows down dynamics in strongly coupled cavities

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Session: Polaritons, July 2, 2024, 10:30 - 12:30

The interplay between kinetic energy and interactions is fundamental in several fields in physics as it stands as the basis for several strongly correlated quantum many-body phenomena such as Wigner crystallization, the fractional quantum Hall effect and Moir´e-related physics. Besides inspiring analogies among diverse physical fields, the ability to control on demand the kinetic energy is highly attractive in photonics because they allow unconventional light flows such as slow-light. Here, we realize room-temperature slow-light with Frenkel polaritons excited across two strongly coupled cavities. We demonstrate the formation of a tuneable heavy-polariton appearing in absence of a periodic in-plane potential. Our simple photonic architecture enables the unique spatial segregation of photons and excitons in different cavities and maintains a balanced degree of mixing between them. This unveils a dynamical competition between many-body scattering processes and the underlying polariton nature which leads to an increased fluorescence lifetime. The polariton features are further revealed under appropriate resonant pumping, where we observe suppression of the polariton fluorescence intensity.

Interplay of flat bands and higher order Van Hove singularities in Kagome metals

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Session: 2D Materials 1, July 3, 2024, 10:30 - 12:40

The Kagome lattice offers a rich platform for the investigation of a plethora of quantum phenomena ranging from frustrated magnetism to superconductivity and flat band physics. In this talk, I will focus on some of the tuneable and non-trivial aspects of the electronic band structure of Kagome metals. Using a series of tight-binding models that are differentiated by the underlying symmetry groups and the types and orders of the hopping parameters, I will demonstrate how symmetry and tuning play an important role in the emergence of flat bands and higher order Van Hove singularities in the band structure of Kagome metals. In this context, I will also introduce a new flat-band score that can be readily applied to tuneable models. This can aid us in engineering optimally flat bands near the Fermi level of quantum materials.

Material with Random Layer Lattice - A State between the Crystalline and Amorphous States

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Session: New Materials 1, July 2, 2024, 10:30 - 12:30

Logically, there should be intermediate states between the 3D-periodical crystalline phase and random amorphous phase. J.D.Bernal had a vision of generalized crystallography long time ago. The discovery of quasi-crystal shed light on this gray zone, A.L.Mackay believed that quasi-crystal presents an intermediate state between the periodic behavior and chaos of dynamic systems in the time domain. In the spatial domain, there are three other dimensions to play with. As earlier as in 1941, B. E. Warren has proposed such one kind of theoretical intermediate state in the spatial domain, which was named as “Random layer Lattice”.

Generally, intermolecular forces are the main driven-force for the phase of materials. To introduce randomness to one specific dimension in the crystal lattice, the key is to weaken the intermolecular force along this dimension to an extreme. The coordination frameworks have provided great freedom for the design of material structure. Here, by using bicyclocalix[2]arene[2]triazine cage molecule as a building block, we have successfully weakened the interlayer interaction to an extreme in the resulting self-assembly lattice. A series of materials with the practice Random layer lattice were prepared in large batch with high yield. The mechanism study identified that the solvent plays a key role to stabilizing the 3D lattice, the de-solvation process caused great decrease of the interlayer interaction, and a dimensional reduction phase transition was observed in this process. This kind of materials can serve as good precursors for mass production of two-dimensional materials. They can also be used as super-lubricating materials.

Unraveling the influence of polarized terminations on the surface states of YbB6 using STM

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Session: Surface Physics, July 5, 2024, 10:30 - 12:30

YbB6 is a predicted topological insulator, with experimental evidence for conducting surface states of yet-unproven origin. However, its lack of a natural cleavage plane, and resultant surface-dependent polarity, has obscured its study. We use scanning tunneling microscopy to image the cleaved surface of YbB6, exhibiting several coexisting terminations with distinct atomic structures. Our spectroscopic measurements show band-bending between the terminations, resulting in both conducting and fully-gapped regions. In the conductive regions, we observe spectral peaks that are suggestive of van Hove singularities arising from Rashba spin-split quantum well states. The insulating regions rule out the possibility that YbB6 is a strong topological insulator, while the spin-polarized conducting regions suggest possible utility for spintronic devices.

Nanomagnet-induced Synthetic Spin-Orbit Coupling in a Superconductor-Semiconductor Nanowire

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Session: Magnetism 3, July 4, 2024, 10:30 - 12:30

Inhomogeneous magnetic fields generated by nanomagnet arrays are predicted to induce a synthetic spin-orbit coupling (s-SOC) in hybrid superconductor-semiconductor nanowires commonly used in the search for Majorana bound states [1]. By obviating the need for intrinsic SOC, nanomagnets could thus widen the range of materials available for realising topological superconductivity, for instance to include lower-disorder materials such as carbon nanotubes or silicon nanowires. Here we present conductance measurements of a proximitized Al/InAs nanowire fabricated adjacent to an array of nanomagnets. In the Coulomb-blockade regime we observe tunnelling resonances at low source-drain bias consistent with the presence of sub-gap Andreev bound states [2]. Using a sequence of externally applied fields to switch the nanomagnets, we verify the expected shift in bound state energy between the anti-aligned and aligned nanomagnet configuration. Our results are consistent with quantum transport simulations and demonstrate the viability of using local magnetic textures to induce s-SOC in hybrid superconductor-semiconductor devices.

[1] Kjaergaard et al., Phys. Rev. B 85, 020503(R) (2012)

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What is the origin of the specific heat capacity of the spin-liquid candidate Ca_{10} Cr_{7} O_{28}?

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Session: Magnetism 1, July 2, 2024, 10:30 - 12:40

Ca_{10} Cr_{7} O_{28} is a promising spin-liquid candidate that has been studied by various groups over the past decade. Seven years ago a model for its magnetism was proposed by Balz et al. The model has been adopted by the community, appearing in many recent theoretical studies on the material. In this talk we will put forward evidence that this currently accepted theory cannot be correct. The basis of the argument is that the magnetic specific heat capacity of the model shows significantly different characteristics to that of the material. We have calculated the former using a complementary set of numerical methods for approximating low temperature thermodynamics including Thermal Pure Quantum States and the High Temperature Expansion. We will then discuss our recent work on modifications to the model with a particular focus on how our knowledge of the chemical structure can be used to refine the otherwise bewildering model-space.

Discovery of Dynamical Heterogeneity in a Magnetic Monopole Fluid

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Session: Strongly Correlated, July 3, 2024, 14:00 - 16:10

Dynamical heterogeneity, in which transitory local fluctuations occur in the conformation and dynamics of constituent particles, is believed universally essential for the evolution of supercooled liquids into the glass state. Yet its microscopic spatiotemporal phenomenology has remained unobservable in virtually all supercooled glass forming liquids. New opportunities to address these issues emerge from recent theoretical advances predicting that dynamical heterogeneity should also occur in supercooled magnetic monopole fluids.

Motivated thus, we searched for the emergence of dynamical heterogeneity when entering the supercooled monopole fluid of Dy2Ti2O7. By measuring microsecond-resolved magnetization noise $\boldsymbol{M(t,T)}$ at temperatures between $\mathbf{15\ mK} < \boldsymbol{T} < \mathbf{3000\ mK}$ we discover a sharp bifurcation in monopole noise characteristics beginning at $\boldsymbol{T} \approx \mathbf{1500\ mK}$, with the appearance of intense monopole current bursts whose magnitude and statistics evolve rapidly with falling temperature. This unique new form of dynamical heterogeneity first emerges upon entering the supercooled monopole fluid regime, reaches maximum intensity near $\boldsymbol{T} \approx \mathbf{500\ mK}$ and then terminates along with coincident loss of ergodicity near $\boldsymbol{T} \lesssim \mathbf{250\ mK}$.

Surprisingly, low intensity, frequency independent, monopole noise persists below $\boldsymbol{T} \lesssim \mathbf{250\ mK}$, representing activity at approximately $\mathbf{2}$% of the Dy sites. Its survival to lowest temperatures $\boldsymbol{T} \lesssim \mathbf{20\ mK}$ reveals a population of quantum dynamical monopoles apparently trapped within the spin-ice ground state. This phenomenology greatly expands our knowledge and understanding of supercooled monopole fluids and, more generally, of the fundamental vitrification process.

Simulating 2D electronic spectroscopy with tensor networks

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Session: Ultrafast/2D, July 5, 2024, 10:30 - 12:40

2D electronic spectroscopy (2DES) is an experimental tool that can image how energy excitations evolve in time with femtosecond resolution. This makes 2DES a powerful technique for investigating quantum mechanical processes in real time, such as the transport of energy in light-harvesting molecules.

In general, these types of quantum systems never exist in isolation, but are coupled to some larger vibrational environment that will affect the dynamics of the system. 2DES had yielded key insights into such environment-mediated processes in light-harvesting materials. However, realistic environments are often non-Markovian, meaning that they retain a memory of their interactions with the system. This makes simulating 2DES measurements challenging and efficient methods that include non-Markovian effects are still lacking.

I will present a tensor network method that can simulate 2DES spectra in a numerically exact way. Our method involves the computation of a process tensor, which efficiently captures the influence of a vibrational environment on the system. A process tensor is the most general representation of an environment that allows one to calculate the effect of applying a measurement on the system at any time point. Our method provides a novel way to extract the information required to model 2DES spectra and provides a new avenue for the application of process tensors.

Universality of intra-unit-cell Cooper-pair modulation

Matteo Dürrnagel[1,2], Hendrik Hohmann[1], Tilman Schwemmer[1], Tobias Müller[1], Xianxin Wu[3], Jia-Xin Yin[4], Ronny Thomale[1]

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Session: Superconductivity 3, July 4, 2024, 10:30 - 12:40

In unconventional superconductors electrons bind over finite distances to form non-trivial angular momentum states in order to orthogonalise the short-ranged screened Coulomb repulsion. Here we report on the theoretical prediction of a superconducting state, whose Cooper-pairs acquire finite angular momentum in the center of mass coordinate [1]. This results in a spatial modulation of the Cooper-pair density, that breaks rotational symmetry within the unit-cell but retains translational invariance of the crystal lattice. We refer to this state as sublattice modulated superconductor (SMS). This novel superconducting phase is distinct from a pair density wave but shares similar phenomenology. Recent experimental progress in high resolution STM studies revealed sublattice modulated superconducting order in kagome [2] and iron-pnictide systems [3] suggesting its existence in other correlated materials like the cuprates or heavy-fermion compounds, where it can be contextualized with the long sought after pair density wave order.

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[2] H. Deng, H. Qin, G. Liu, T. Yang, et. al. Chiral kagome superconductivity modulations with residual Fermi arcs. submitted. (2024).
[3] L. Kong, et. al. Observation of Cooper-pair density modulation state. arXiv:2404.10046. (2024).

Driving Viscous Hydrodynamics in Bulk Electron Flow in Graphene Using Micromagnets

Jack Engdahl[1], Dr Aydin Cem Keser[2], Prof Oleg Sushkov[1], Dr Thomas Schmidt[3,4]
[1]UNSW, Australia, [2]CSIRO, Australia, [3]University of Luxembourg, Luxembourg, [4]Victoria University of Wellington, New Zealand
Session: 2D materials 2, July 4, 2024, 14:00 - 16:00

We consider the hydrodynamic flow of an electron fluid in a channel formed in a two-dimensional electron gas
(2DEG) with no-slip boundary conditions. To generate vorticity in the fluid, the flow is influenced by an array
of micromagnets on the top of the 2DEG. We analyze the viscous boundary layer, and we demonstrate anti-Poiseuille behavior in this region. Furthermore, we predict a longitudinal voltage modulation, where a periodic
magnetic field generates a voltage term periodic in the direction of transport. From an experimental point of view,
we propose a method for a boundary-independent measurement of the viscosity of different electron fluids. The
results are applicable to graphene away from the charge-neutrality point and to semiconductors.

Metal 3D Printing of Nb-47Ti Superconductor Components

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Session: Thin Films, July 5, 2024, 10:30 - 12:30

Metal 3D printing of superconductors may provide a more economical manufacturing route that can produce complex superconductor components for advanced applications, including quantum computers, magnetic shields, magnetic resonance imaging, and superconducting radio frequency (SRF) cavities. In this study, Nb-47Ti superconducting alloy was fabricated using Laser Powder Bed Fusion (LPBF), a low-cost approach that involves blending elemental powders of Nb and Ti, then using the laser to fully homogenize the two elements to in-situ create the alloy structures. The process parameters were optimized for maximum microstructural density and lowest Nb segregation. Post-processing heat treatments were applied to homogenize the microstructure by dissolving the remaining Nb particles throughout the matrix. Additional aging treatments were also performed and optimized according to the differential scanning calorimetry measurements to generate the necessary α-Ti precipitates that act as pinning centers for the fluxoids to improve the superconductivity. Electrical and magnetic properties were measured to assess the optimum heat treatment cycle in terms of superconducting properties. The thermal variation of electrical resistivity showed a critical temperature (Tc) value of 9.9K for the optimized heat-treatment condition. The critical current density (Jc) was calculated using Bean's model employing the magnetic hysteresis loops, giving a value of 14.7 kA/mm² (at 4.2K, 5T) for the best case. Eventually, the optimized process cycle for in-situ alloying NbTi superconductors via LPBF was used to manufacture an SRF cavity. The advantages and limitations of this approach will be discussed.

Bad Weyl semimetals and spinon Fermi arcs in a model for pyrochlore iridates

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Session: Magnetism 2, July 2, 2024, 14:00 - 16:00

The Weyl-Mott insulator (WMI) has been postulated as a novel type of correlated insulator with nontrivial topological properties. We introduce a minimal microscopic model that captures generic features of the WMI transition in Weyl semimetals. The model hosts a bulk Mott insulator with spinon Fermi arcs on its surfaces which we identify as a WMI, i.e., a U(1) Weyl quantum spin liquid. At finite temperatures, we find an intermediate Weyl semimetallic phase with no quasiparticles which is consistent with the bad semimetallic behavior observed in pyrochlore iridates, $A_2Ir_2O_7$, close to the Mott transition. Spinon Fermi arcs lead to a suppression of the bulk Mott gap at the surface of the WMI, in contrast to the gap enhancement expected in conventional Mott insulators, which can be detected through angular resolved photoemission spectroscopy.

Numerical evidence for weak and "half-weak" first-order phase transitions in the frustrated classical J1-J2 square lattice Ising model

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Session: Magnetism 3, July 4, 2024, 10:30 - 12:30

The phase boundaries of the frustrated classical Ising model on the square lattice with nearest- and next-nearest-neighbour couplings have eluded complete understanding in spite of decades of numerical effort. A recent study [1] approaches this problem in a previously untried way: adiabatic evolution of tensor networks. In this talk we review the following results from this study that shed new light on this very old problem:

1) The current consensus is that the phase boundary is second order in the region J2/|J1|>0.67, however we find strong evidence that the entire phase boundary is first-order in the region J2/|J1|>0.5 such that it only asymptotically becomes second order in the limit J2/|J1|-> infinity.

2) As J2/|J1|->0.5^+, we find suggestive evidence that the phase boundary becomes of a first-order character that is neither weak first-order (i.e., very large correlation lengths in both coexisting phases at the phase boundary) nor strong first-order (i.e., very small correlation lengths in both coexisting phases at the phase boundary) but instead "half-weak" first-order (i.e., a very large correlation length in one of the coexisting phases and a very small correlation length in the other coexisting phase at the phase boundary).

[1] A. A. Gangat, Phys. Rev. B 109 (10), 104419 (2024)

Quantum nanoelectronics at ultrafast time scales

Dr. Giorgos Georgiou[1], Dr. Christopher Bauerle[2], Dr. Clement Geffroy[2], Mr. Thomas Vasselon[2], Mr. Matteo Aluffi[2], Mr. Seddik Ouacel[2]
[1]University Of Glasgow, United Kingdom, [2]Institute NEEL, CNRS, France

Session: Materials for Quantum Technologies 2, July 4, 2024, 10:30 - 12:30

Quantum transport of electrons in nanoelectronic devices has long been studied using DC streams of electrons. As nanoelectronic devices become smaller and smaller, quantum mechanical effects and multi-electron interactions become more relevant. In this talk, I will discuss the state-of-the-art research in ultrafast quantum nanoelectronics, where picosecond-duration electron wavefunctions, also known as Levitons, are injected in quantum nanoelectronic devices.
Electron transport at these ultrafast time scales offers a rich playground where fundamental effects can be studied. By using frequency comb-based voltage sources, we create electron wavefunctions as short as 30ps and we are able to reconstruct in-situ the electron wavefunction. The electronic excitations are then transported over long distances and we study the propagation characteristics. These ultrashort electron wavefunctions can be used to directly investigate real-time dynamics of electron-electron interaction phenomena in low-dimensional conductors.

Fully-gapped superconductivity in quasi-1D spin-triplet candidate Li0.9Mo6O17

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Session: Superconductivity 2, July 3, 2024, 14:00 - 16:10

Quasi one-dimensional lithium molybdenum purple bronze Li0.9Mo6O17 (LMO) is a leading candidate for the realisation of a Tomonaga-Luttinger liquid (TLL) ground state in addition to exhibiting emergent symmetry at low temperature [1,2]. Superconductivity emerges in this system at Tc ≈ 2.3 K, with the upper critical field along the conductive axis, Hc2 ≈ 15 T, exceeding the Pauli paramagnetic limit, possibly indicative of an unconventional spin-triplet pairing state [3]. Until now, however, no further studies of the symmetry and structure of the superconducting order parameter have been conducted, and the origin of the pairing in LMO has remained elusive.
We have performed magnetic penetration depth measurements using a tunnel-diode oscillator technique down to 70 mK, and specific heat measurements down to 300 mK, to probe the low-energy quasiparticle excitations in the superconducting state. Our investigations reveal that the pairing state is fully-gapped at all points on the Fermi surface, and obtain a relatively small gap minimum, $\Delta \approx 0.3\ k_B T_c$, from activated exponential behaviour. In contrast, the large specific heat anomaly observed suggests a strong-coupling scenario which is associated with a larger gap. We therefore infer that the gap structure of LMO is highly anisotropic. These results are discussed in terms of the possible pairing symmetries and microscopic models.

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Spin Coherence of the Clock Molecule 15N@C60

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Session: Materials for Quantum Technologies 2, July 4, 2024, 10:30 - 12:30

The endohedral fullerene $^{15}N@C_{60}$ has a spin resonance transition at ~38.6 MHz which is independent of magnetic field to first-order and is therefore suitable as a frequency reference for an atomic clock [1]. This may be implemented in a chip-scale condensed matter atomic clock operating at room temperature.

The potential stability of such a clock depends on the spin coherence time, which determines the sharpness of the reference transition. At microwave frequencies $^{15}N@C_{60}$ has one of the longest coherence times of any molecule [2], however the coherence time at the radio frequency clock transition is unknown.

We have measured the spin coherence time of this material at low frequencies approaching the clock transition using pulsed spin resonance. In contrast to previous non-pulsed measurements, this allows us to extract the true quantum coherence time T2. From these results, we will estimate the accuracy of a future $^{15}N@C_{60}$ atomic clock.

References:

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Surface structure of the strontium ruthenates

Daniel Halliday[1,2], Dr Georg Held[2], Dr Luke C. Rhodes[1], Professor Peter Wahl[1], Professor Phil D. C. King[1]
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Session: Surface Physics, July 5, 2024, 10:30 - 12:30

The intertwined nature of spin, charge, orbital and lattice degrees of freedom in strongly correlated electron materials leads to emergent orders highly responsive to external stimuli [1]. In the ruthenium oxides, subtle structural variations of the RuO6 octahedra induce significant changes in physical properties. For example, substituting Sr with Ca in Ca2-xSrxRuO4 yields a diverse phase diagram with metallic, Mott insulating, and superconducting phases, where the dominant structural change to the material is a rotation and tilting of the RuO6 octahedra [2]. Interestingly, surface relaxations of the ruthenium oxides enable the realization of distinct ground states in the surface layer [3-5]. To elucidate the relationship between structural details and electronic structure, accurate determination of surface relaxation and potential reconstruction is crucial. Low energy electron diffraction (LEED) provides insights into small structural distortions at the surface layer, facilitating a quantitative understanding of their impact on quantum many-body states. We apply LEED to the n=1-3 members of the strontium ruthenate family (Srn+1RunO3n+1), reporting new temperature-dependent LEED-I(V) measurements to constrain structural distortions and search for structural transitions of the surface layer. By examining structural distortions within the surface layer our findings contribute new insights for modelling and understanding of the electronic structure near the Fermi energy.

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Low-energy spin fluctuations in the strange metal state of an overdoped cuprate superconductor

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Session: Superconductivity 1, July 2, 2024, 14:00 - 16:00

Theories of the origin of superconductivity in cuprates are dependent on an understanding of their normal state which exhibits various competing orders. Transport and thermodynamic measurements on La2-xSrxCuO4 show a peak in the electronic specific heat C versus doping p, near the doping p* where the pseudogap collapses. Here we use inelastic neutron scattering to show that close to Tc and near p*, there are very-low-energy collective spin excitations with characteristic energies $\hbar\Gamma \approx 5$ meV. Cooling and applying a 8.8 Tesla magnetic field creates a mixed state with a stronger magnetic response below 10meV. We conclude that the low-energy spin-fluctuations are due to the collapse of the pseudogap combined with an underlying tendency to magnetic order. We show that the large specific heat near p* can be understood in terms of collective spin fluctuations.

QUEST-DMC: Modelling early-Universe phase transitions in superfluid helium-3 under nanofluidic confinement

Dr Petri Heikkinen[1], Dr Lev Levitin[1], Mr Nathan Eng[1], Dr Xavier Rojas[1], Dr Angadjit Singh[1,2], Dr Samuli Autti[3], Prof Richard Haley[3], Prof Mark Hindmarsh[4,5], Dr Kuang Zhang[4,5], Dr Dmitry Zmeev[3], Prof Jeevak Parpia[6], Prof Andrew Casey[1], Prof John Saunders[1]

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Session: Topology, July 2, 2024, 10:30 - 12:30

The mechanism behind the first-order phase transition between the chiral A and time-reversal-invariant B phases of superfluid ^{3}He has evaded explanation despite decades of both experimental and theoretical work. Cosmological analogues connect this fundamental problem of condensed matter physics with the possible early-Universe phase transitions and associated generation of gravitational waves, predicted in many extensions of the Standard Model of particle physics.

The A-to-B phase transition can be triggered extrinsically by ionising radiation or heterogeneous nucleation arising from the details of the sample container. However, the role of potential cosmologically relevant homogeneous intrinsic nucleation mechanisms remains elusive, with the existing models based on both thermal fluctuations and quantum tunnelling predicting a lifetime of the supercooled ^{3}He-A longer than the age of the Universe.

Within the QUEST-DMC project, we have nanofabricated a novel silicon stepped-height sample container with five 6.8 μm deep phase-transition chambers. Close to atomically smooth walls together with a 75 nm deep isolation barrier surrounding these chambers ensure protection against any obvious sources of heterogeneous nucleation. The tiny volumes also ensure that the transitions triggered by ionising radiation are strongly suppressed, providing a versatile platform for exploring both intrinsic and extrinsic phase-transition mechanisms.

Here we report the experimental SQUID-NMR results, showing both strong supercooling of ^{3}He-A and superheating of ^{3}He-B, with stochastic processes dominating the phase transitions between the two. For the first time, we discover a non-monotonic temperature dependence of the lifetime of the supercooled ^{3}He-A. The possible causes of this are discussed.

Topological Hall Effect in Mn3Pt and Mn3Sn

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Session: Magnetism 2, July 2, 2024, 14:00 - 16:00

It is understood that the antiferromagnetic metals Mn3Pt and Mn3Sn show a large Hall effect due to the Berry phase curvature in k-space. Experimental demonstration requires aligning antiferromagnetic domains. That was easier to achieve in Mn3Sn, where a small ferromagnetic moment combined with weak pinning allows antiferromagnetic domains to be aligned with a small applied field [1]. In Mn3Pt, on the other hand, the ferromagnetic moment is undetectably small and pinning is strong. We demonstrate domain alignment by applying uniaxial stress to induce a ferromagnetic moment and applying a field. We show that the Hall effect remains locked in after the stress is removed, confirming that its origin is in the antiferromagnetism [2].

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Hydrodynamics and long-lived modes in two-dimensional Fermi liquids

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Session: 2D materials 2, July 4, 2024, 14:00 - 16:00

There is currently much experimental interest in studying transport in ultraclean two-dimensional materials, which is dominated by electron interactions as opposed to the conventional phonon or impurity scattering. This gives rise to an effective hydrodynamic description of electron flow, with transport coefficients (like the shear viscosity) that can be predicted from an underlying Fermi-liquid description. While one could think that this framework should be extremely well understood, it turns out that there are still fundamental aspects that remain unexplored. In this talk, I will give an introduction to Fermi liquids and hydrodynamic transport in 2D materials, and discuss how Pauli blocking gives rise to excitations with lifetimes that are much longer than conventionally expected in Fermi liquid theory. I will discuss the possible signatures of these modes in transverse sound and nonlinear thermal transport.

Non-Fermi Liquids Arising from Magnetic Field Interactions: A Functional Renormalisation Group Analysis

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Session: Strongly Correlated, July 3, 2024, 14:00 - 16:10

We use the functional renormalisation group (fRG) to study finite-density electrons interacting with a dynamic magnetic field. The magnetic vector potential is not screened by the particle-hole continuum and thus mediates singular interactions between electrons, which can cause the quasiparticle weight to vanish [1]. Most techniques previously used on this problem [1-3] are perturbative; fRG, by contrast, is non-perturbative, and so can better handle the strong interactions and non-analytic operators inherent to non-Fermi liquids. Using an ansatz for the effective action that respects gauge symmetry at all scales, we obtain and discuss the resulting non-Fermi liquid fixed point and how its properties depend on dimensionality. We comment on the UV-IR mixing exhibited by the low-energy physics due to gauge symmetry, and the implications our results have for predictive modelling of non-Fermi liquids.

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[3] Y. B. Kim, A. Furusaki, X.-G. Wen and P. A. Lee, Phys. Rev. B 50, 17917 (1994).

Quantum walk algorithms for finding spin glass ground states

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Session: Materials for Quantum Technologies 3, July 4, 2024, 14:00 - 16:00

Works by Callison et al (2019) and Montanaro (2019) have shown that quantum algorithms based on quantum walks can find spin glass ground states more efficiently than classical algorithms. We extend this work to multi-stage quantum walks, in which a sequence of quantum walks with different hopping rates is applied (without intermediate measurements). The hopping rates can be chosen to maximise the probability of finding the ground state: in the limit of many stages this is equivalent to adiabatic quantum state transfer, and can find the ground state with near certainty for gapped systems. We critically examine the distinctions between algorithms which approximate the ground state (with bounded error) and those which guarantee the output is the true ground state. Our work has wider implications for efficiently simulating quantum systems using hybrid quantum-classical algorithms.

Cavity electrodynamics of van der Waals heterostructures

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Session: Polaritons, July 2, 2024, 10:30 - 12:30

Van der Waals (vdW) heterostructures host many-body quantum phenomena that can be tuned in situ using electrostatic gates. These gates are often metallic graphite flakes and only tens of microns in size. In this talk we show, that these flakes naturally form plasmonic THz cavities, that operate on the same µeV - meV energy scale as the phenomena they electrically control. Using on-chip THz spectroscopy, we captured the sub-wavelength cavity electrodynamics of a vdW material, graphene, and its graphite gate. We observe spectral weight transfer and the formation of an avoided crossing between the graphite cavity mode and graphene plasmon modes as the graphene carrier density was tuned. The magnitude of the avoided crossing was found to be in the ultrastrong coupling regime, where photon vacuum fluctuations may be sufficient to manipulate matter. Our findings show that built-in cavity modes of metallic gates could manipulate low-energy electrodynamics of vdW heterostructures. This opens a pathway for deeper understanding of emergent phases in these materials and new functionality through cavity control.

Non-ergodicity of nuclear spins in a dilute system of two dimensional 3He impuritons

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Session: Non-equlibrium and Quantum Thermodynamics, July 3, 2024, 14:00 - 16:10

The inability of low dimensional quantum systems with quenched randomness to thermalize is both of fundamental interest and of relevance to the operation of quantum devices. Here we report results on a low density of substitutional ^{3}He impurities (impuritons) in the second layer of an adsorbed double layer film of ^{4}He on graphite. Such impuritons can quantum-tunnel by exchange with ^{4}He atoms within the second layer, subject to the periodic potential of the first layer and ^{3}He-^{3}He strain mediated interactions. Our experimental probe is magnetic resonance on the ^{3}He nuclear spin, in which we observe saturation curves under a repeated train of relatively small-angle tipping pulses. A striking observation is anomalous spin–lattice relaxation, with a very broad distribution of T_1, which is strikingly spiked around the 7/12 commensurate density. At this total density, the ^{3}He impurities can occupy three distinct sites. The T_1 distribution extends over five orders of magnitude. The form of the distribution is temperature independent, but characterised by a time T_1† which increases from 0.1s to 10^4s on cooling from 50 mK to around 1 mK. These properties indicate an inability of sub-systems to thermalize, signalling the absence of diffusion induced by disorder and strain interactions, characteristic to the phenomenon of many-body localisation.

Deterministically induced single-photon light emitting diodes

Dr Aleksey Kozikov[1], James Howarth[2], Kristina Vaklinova[3], Magdalena Grzeszczyk[3], Giulio Baldi[3], Lee Hague[2], Marek Potemski[4], Kostya Novoselov[3], Maciej Koperski[3]

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Session: Materials for Quantum Technologies 2, July 4, 2024, 10:30 - 12:30

We reliably create single photon emitters (SPEs) in transition metal dichalcogenides at specific locations, on demand, via nanopillar imprinting and helium ion irradiation. We realise atomically thin vertical tunnelling light-emitting diodes based on WSe2 monolayers with deterministically induced SPEs. We investigate the evolution of their emission spectra in external electric and magnetic fields, and demonstrate significant tuneability of their emission energy.

SPEs are fundamental building blocks in quantum information technologies. Novel two-dimensional (2D) materials show promise in this field of research due to their atomically thin nature and the ability to transfer them reliably to any substrate, even in ambient conditions using van der Waals transfer techniques. Two of the significant challenges in integrating SPEs into 2D materials in photonic circuits include difficulties in precisely locating SPEs and in electrically controlling their emission. Deterministically induced and electrically controllable SPEs are crucial for the development of future quantum optical devices.

Nature of Topological Phase Transition of Kitaev Quantum Spin Liquids

Frank Kruger[1], Huanzhi Hu
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Session: Topology, July 2, 2024, 10:30 - 12:30

We investigate the nature of the topological quantum phase transition between the gapless and gapped Kitaev quantum spin liquid phases away from the exactly solvable point. The transition is driven by anisotropy of the Kitaev couplings. At the critical point the two Dirac points of the gapless Majorana modes merge, resulting in the formation of a semi-Dirac point with quadratic and linear band touching directions. We derive an effective Gross-Neveu-Yukawa type field theory that describes the topological phase transition in the presence of additional magnetic interactions. We obtain the infrared scaling form of the propagator of the dynamical Ising order parameter field and perform a renormalization-group analysis. The universality of the transition is found to be different to that of symmetry-breaking phase transitions of semi-Dirac electrons. However, as in the electronic case, the Majorana fermions acquire an anomalous dimension, indicative of the breakdown of the fractionalized quasiparticle description.

Synthesis, Electronic and Magnetic Investigation of Polymorphic 2D CrxTey Monolayers

Naina Kumari[1,2], Phil King[1], Charlotte Sanders[2], Akhil Rajan[1], Brendan Edwards[1], Liam Trzaska[1], Sebastian Buchberger[1], Yoshiko Nanao[1]

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Session: Thin Films, July 5, 2024, 10:30 - 12:30

Two-dimensional (2D) materials host diverse electronic and magnetic properties. Exploring electronic states in 2D systems offers insights distinct from those observed in bulk materials [M. Gibertini et al., Nat. Nanotechnology 14 (2019)]. Notably, 1T-CrTe2 stands out, displaying room temperature ferromagnetic behaviour in bulk. However, it is only metastable, readily decomposing into self-intercalation compounds [Kinga Lasek et al., ACS Nano 14 (2020)].

We present the systematic growth of monolayer 1T-CrTe2 and Cr2Te3 using molecular beam epitaxy. These share a similar crystal symmetry, but with the later being effectively a bilayer of CrTe2 with additional Cr intercalated within the van der Waals gap. Our observations highlight the critical role of low growth temperatures (Ts) in stabilising the metastable CrTe2 phase, which undergoes a structural phase transition (Cr1+xTe2) with Cr-intercalation at elevated Ts. We further demonstrate how the growth rate and quality can be enhanced by using Ge as a surfactant during growth. Using angle-resolved photoemission spectroscopy (ARPES), we demonstrate distinct electronic properties of the stabilised polymorphs, with metallic behaviour for 1T-CrTe2 and semiconductor-like behaviour for Cr2Te3. Corresponding hysteresis loops derived from X-ray magnetic circular dichroism signal peak intensities confirm the ferromagnetic nature of Cr2Te3 but signify a weak paramagnetic-like response for CrTe2. However, from temperature dependent ARPES for CrTe2 we find a clear band-shift, confirming a magnetic phase transition and suggesting its antiferromagnetic nature.

Our findings offer insight into the self-intercalated structural phase transition of the metastable phase, relevant for spintronics applications [Ethan et al., npj 2D materials and application 4 (2020)].

Kernel Polynomial Method for Linear Spin Wave Theory

Dr Harry Lane[1], Hao Zhang, David Dahlbom, Sam Quinn, Rolando Somma[2], Martin Mourigal, Cristian Batista, Kipton Barros

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Session: Magnetism 1, July 2, 2024, 10:30 - 12:40

The calculation of dynamical correlations in magnetic systems is a key component of matching spectroscopic measurements to model spin Hamiltonians. Linear spin wave theory has become one of the most powerful methods to perform such calculations and is used extensively in momentum-resolved measurement techniques such as inelastic neutron scattering. However, for large system sizes, the diagonalisation of the dynamical matrix becomes a numerical bottleneck. This limits the utility of linear spin wave theory for a large range of systems of extreme experimental interest, such as disordered, incommensurate, and multi-Q systems. In this talk, we introduce an efficient scheme for the calculation of dynamical correlations, with broad applicability to numerous spectroscopic probes. This method reduces the computational complexity from cubic to linear in system size. We demonstrate the power of this approach by applying it to calculations of the neutron scattering response of incommensurate, skyrmion lattice and disordered magnetic systems. We suggest that this approach will allow for the inverse modelling of complex systems with large magnetic unit cells.

Majorana or not? A story of Fe(Se,Te)

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Session: Superconductivity 3, July 4, 2024, 10:30 - 12:40

The search for Majorana fermions in condensed matter systems has resulted in a number of putative claims of their discovery. If true, these exotic particles, that are their own anti-particle, could become the basis for error-free quantum computing. Unambiguous proof, however, is thus far lacking and challenging to provide. A recently proposed method to distinguish Majorana bound states from more conventional Andreev-, and Yu-Shiba-Rusinov states is to measure their shot noise [1]. Using our MHz enabled scanning tunnelling microscope [2], we set out to investigate two possible Majorana sightings in Fe(Se,Te): zero energy bound states at single Fe impurities and linear sub-gap density of states at 1D defects. In this talk I will discuss our findings.

[1] Phys. Rev. B 104, L121406 (2021)
[2] Rev. Sci. Instrum. 89, 093708 (2018)

One-dimensional Z4 topological superconductor

Max Tymczyszyn[1], **Edward McCann**[1]
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Session: Electronic Structure 2, July 4, 2024, 10:30 - 12:30

We describe the mean-field model of a one-dimensional topological superconductor with two orbitals per unit cell. Time-reversal symmetry is absent, but a nonsymmorphic symmetry, involving a translation by a fraction of the unit cell, mimics the role of time-reversal symmetry. As a result, the topological superconductor has Z4 topological phases, two which support Majorana bound states and two which do not, in agreement with a prediction based on K-theory classification [K. Shiozaki et al., Phys. Rev. B 93, 195413 (2016)]. As with the Kitaev chain, the presence of Majorana bound states gives rise to the 4π-periodic Josephson effect. We discuss the role of disorder and the relation of this model to models in other symmetry classes with nonsymmorphic symmetries.

Modification of surface phenomena at hybrid Bi2Se3/organic interfaces

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Session: Hybrid Organic/Inorganic, July 3, 2024, 10:30 - 12:40

Topological insulators such as Bi_2Se_3 have interesting transport properties, including undamped electronic transport via topologically-protected surface states. Manipulation of surface plasmons has been previously demonstrated using magnetic dopants, but these cannot be altered after growth. In contrast, the use of organic molecular overlayers such as C_{60} could be advantageous because it is possible to 'gate' the C_{60} interaction through electrical biasing and thereby develop tunable devices. Here, we investigate plasmonic interactions at the interface of an as-deposited thin film sample of Bi_2Se_3/C_{60} using electron energy loss spectroscopy (EELS).

We will show the observation of a surface plasmon from Bi_2Se_3 at 5 eV, localised to the Al_2O_3/Bi_2Se_3 interface. Its plasmon dispersion, obtained using momentum-resolved EELS, was observed to follow an almost linear trend, similar to that predicted for π-electrons in graphene[1] suggesting the presence of a strongly confining interfacial potential. Comparison with simulations suggests that the nature of this surface plasmon could be a result of Bi_2Se_3 π-electrons confined in 2D to the surface[1]. With crystalline C_{60} present, the surface plasmon energy was shifted higher with a similar dispersion trend. Through the introduction of organic molecules such as C_{60}, a strongly 2D-confined surface mode at the interface with Bi_2Se_3 was observed. In conclusion, unusual plasmon dispersion of the Bi_2Se_3 surface plasmon was observed with similar dispersion to 2D π-electrons in graphene and upon contact with C_{60} its energy was shifted. This phenomenon in the as-deposited sample could be controlled through gating for development of plasmonic devices.

[1]Liou,S.C. et al.(2015)Physical Review B,91(4),pp.045418.

From matrix product states to field theory in the J1-J2 spin chain

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Session: Magnetism 3, July 4, 2024, 10:30 - 12:30

We study the J_1-J_2 spin-1/2 chain using a path integral constructed over matrix product states (MPS). By virtue of its non-trivial entanglement structure, the MPS ansatz captures the key phases of the model even at a semi-classical, saddle-point level, and, as a variational state, is in good agreement with the field theory obtained by abelian bosonisation.

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

Large Spin Hall Angle in Mn-based Antiferromagnetic Alloys

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Session: Magnetism 2, July 2, 2024, 14:00 - 16:00

Historically, antiferromagnets (AFM) were believed not to exhibit any anomalous Hall conductivity (AHC). Conversely, ferromagnets have long been known to exhibit AHC and, therefore, to show a transverse voltage without the need for a magnetic field since the discovery by Edwin Hall in 1881. Recently, however, it was shown that some AFMs can indeed manifest AHC. Furthermore, AFMs could serve as promising components for next-generation spintronics devices, thanks to their scalability, robustness against external magnetic fields, and ultrafast spin dynamics.
In this theoretical work, we employ density functional theory and Green's function methods to calculate the transport properties of Mn-based binary alloyed AFMs, specifically focusing on the total spin Hall conductivity (SHC), incorporating both the intrinsic contribution due to the Berry curvature, and the extrinsic contributions arising from skew scattering and side-jump processes. Our goal is to identify a suitable AFM for spintronic applications that exhibits a high spin Hall angle (SHA); with an efficient charge-to-spin Hall conductivity conversion ratio.
Our findings indicate that doping MnPt with Pd (MnPtx Pd1 – x) can significantly increase the SHA from approximately 2% to 5%. This enhancement should be experimentally observable, particularly at room temperature where the effect is further amplified, resulting in the SHA reaching around 8%. In the case of the MnPtx Ir1–x alloy, we observe even more impressive results, with SHA reaching up to 13% at room temperature. These results suggest that antiferromagnetic alloys are promising for efficient spin current generation.

Terahertz coherent magnonics in canted antiferromagnets

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Session: Spintronics, July 3, 2024, 14:00 - 16:10

Magnonics aims to employ quanta of spin waves, magnons, to carry, transport and process information, avoiding the dissipation of energy inherent to electronics. Experiments on magnons in regular (ferro)magnets have yielded demonstrations of basic logic devices, albeit macroscopic (mm-scale) in size and operating at GHz frequencies. Recently, the spotlight has shifted towards the use of antiferromagnets, in which neighbouring spins are aligned antiparallel to each other. This alternating order leads to significantly higher spin wave propagation velocities and might enable devices operating at terahertz (trillion of hertz) clock-rates. However, the absence of the net magnetisation also makes antiferromagnets magnetically 'invisible': it is very hard to detect and influence the antiferromagnetic order. Yet, in some antiferromagnets strong spin–orbit coupling results in canting of the spins, thereby producing net magnetization. The canted antiferromagnets combine antiferromagnetic order with phenomena typical for ferromagnets and hold a great potential for spintronics and magnonics. In this way they can be identified as closely related to the recently proposed novel class of magnetic materials, called altermagnets. In my talk I will discuss a new functionality of canted antiferromagnets and altermagnets for magnonics and show that these materials facilitate mechanisms allowing to generate, detect and nonlinearly convert propagating magnons at the nanoscale [1-3].

[1] Hortensius, et al. Nature Physics 17, 1001 (2021);

[2] Leenders and Mikhaylovskiy. Phys. Rev. B 107, 094423 (2023);

[3] Leenders, Afanasiev, Kimel, and Mikhaylovskiy. Nature (in press, 2024).

Breaking the angular dispersion limit in thin film optoelectronics by ultra-strong light-matter coupling

Dr Andreas Mischok[1], Dr Sabina Hillebrandt[1], Dr Bernhard Siegmund[2], MSc Julia Witt[1], Dr Florian Le Roux[1], Dr Seonil Kwon[1], Prof Koen Vandewal[2], Prof Malte Gather[1,3]

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Session: Polaritons 2 and cavity QED, July 2, 2024, 14:00 - 16:00

Thin film interference lies at the core of a multitude of photonic devices. Proper control of thin optical films offers a meticulous handle on the spectral attributes crucial in optoelectronic systems. Microcavities, when undergoing constructive interference, can yield a distinct emission, transmission, or absorption profile. However, the inherent angular dependence of reflection and refraction at film interfaces manifests as pronounced blue shifts at non-normal angles of incidence. To mitigate this effect, we employ ultra-strong coupling between cavity photons and material excitons. Through this coupling, we can transform the photonic to an exciton-like dispersion and effectively flatten the parabolic spectral shift in a wide array of thin-film devices. This approach is particularly potent with organic materials boasting high oscillator strengths, and thus enables angle-independent, narrowband responses within such cavities. We deploy this technique to realize both narrowband as well as broadband transmission filters in simple metallic cavities and further generalise the behaviour to more versatile dielectric stacks with superior performance (1). In optoelectronic devices, we realise polaritonic narrowband photodetectors, and organic LEDs (2,3) with unprecedentedly low dispersion. Spanning the visible to near-infrared spectrum, this paradigm proves adaptable to micro-optics, biophotonics, and other domains grappling with light collimation issues. Our work showcases the versatility and practical utility of strong coupling in creating spectrally pure, color-stable devices for cutting-edge optoelectronics.

1. Mischok, et al. under review (2024).
2. Mischok, et al. Nature Photonics 17, 393 (2023).
3. Witt, AM, et al. ACS Photonics, 10.1021/acsphotonics.3c01610 (in press, 2024).

Topological Classification of Dimensionally Embedded Chains of Magnetic Impurities on Superconductors

Mr Harry Mullineauxsanders[1], Dr Bernd Braunecker[1]
[1] *University Of St Andrews, United Kingdom*

Session: Electronic Structure 2, July 4, 2024, 10:30 - 12:30

A chain of magnetic impurities embedded into an s-wave superconductor bind Yu-Shiba-Rusinov states [1], creating in gap bands that can be tuned through a topological phase transition [2]. The topological classification of this cannot be done through conventional methods, due to the dimensional mismatch and local nature of topological bands bound to the impurity chain. We put forward several methods of classification, providing a proof of the Green's function method proposed in [3], commenting on the applicability of the ground state projector introduced in [4] and study the topological properties of the interaction of YSR bands through the substrate via spectral localiser theory [5].
[1] L. Yu (1965) Acta. Phys. Sin. 21, 75-91; H Shiba (1968) Prog. Theor. Phys. 40, 435-451; A Rusinov (1969) JETP Lett. 9, 85-87
[2] S. Nadj-Perge et al. (2013) PRB 88, 020407
[3] C. Carroll & B. Braunecker (2021) PRB 104, 245133; C. Carroll & B. Braunecker (2021) PRB 104, 245134
[4] T. Tuegel et al. (2019) PRB 100, 115126
[5] T. Loring (2015) Ann. Phys. 356, 383-416; H. Schulz-Baldes & T. Loring (2018) arXiv1802.04517; A. Cerjan & T. Loring (2022) PRB 106, 064109

Quantum transport theory for 2D-topological electronics: translating quantum matter into emerging device paradigms

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Session: Magnetism 2, July 2, 2024, 14:00 - 16:00

This talk concerns quantum transport theory aided explorations on translating topological quantum matter into viable emerging device paradigms [1-2]. First, we present a realizable device design for an all-electrical robust topological valley filter [1] that utilizes spin protected topological kink states hosted on monolayer 2D-Xene materials with large intrinsic spin-orbit coupling. We elucidate the role of spin-orbit coupling in achieving an improved valley filter performance with a perfect quantum of conductance attributed to the topologically protected kink states. We further elaborate clearly the right choice of material, device geometry and other factors that need to be considered for such a functionality [1]. Crucially, we elucidate how gating techniques can be utilized toward realizing “on-demand” topological symmetry protection. We then extend these ideas to propose a topological quantum field-effect transistor (TQFET) that can potentially be engineered to enable sub-thermionic transistor operation coupled with dissipationless ON-state conduction. We finally discuss the applications toward understanding many recent experiments in the rapidly emerging field of spin-valley qubits in bilayer graphene quantum dots [3].

[1] K. Jana and B. Muralidharan, npj 2D Materials and Applications, 6, 19, (2022).
[2] S. Banerjee et.al., Phys. Rev. Applied, 18, 054088, (2022).
[3] A. Mukherjee and B. Muralidharan, 2D Materials, 10, 035006, (2023).

Low dimensional electronic state at the surface of a transparent conductive oxide.

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Session: Surface Physics, July 5, 2024, 10:30 - 12:30

Perovskite alkaline earth stannates, such as BaSnO3 and SrSnO3, showing light transparency and high electrical conductivity (when doped), have become promising candidates for novel optoelectronic devices. Such devices are mostly based on hetero-structures, and understanding their electronic structure, which usually deviates from the bulk, is mandatory for exploring a full application potential. Employing angle-resolved photoemission spectroscopy and ab initio calculations, we reveal the existence of a 2-dimensional metallic state at the SnO2-terminated surface of a 1% La-doped BaSnO3 thin film. The observed surface state is characterized by distinct carrier density and a smaller effective mass in comparison with the corresponding bulk values. The small effective mass of the surface state of about 0.12me warrants that BSO can be an essential ingredient in transition metal oxide heterostructures with a significantly improved electrical conductivity.

Low-temperature in-plane anisotropy of the electrical resistivity in YBa2Cu3O7-δ

Rebecca Nicholls[1], Dr Roemer Hinlopen[2], Dr Jake Ayres[1], Professor Nigel Hussey[1], Professor Antony Carrington[1]

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Session: Superconductivity 1, July 2, 2024, 14:00 - 16:00

The observation of a rapid change in the low-T Hall number n_H(0) from p (the number of doped holes) to 1 + p (the full LDA carrier density) suggests possible critical behaviour near the pseudogap end point (p*) in YBa2Cu3O7-δ (YBCO) [1]. In a more recent study on the single-layer cuprates Tl2Ba2CuO6+δ (Tl2201) and La-doped Bi2Sr2CuO6+δ (La-Bi2201) [2], the evolution from p to 1 + p was instead found to extend toward the edge of the superconducting dome. The inconsistency in experimental trends is sometimes posited to be the consequence of a structural feature found only in YBCO. In YBCO, quasi-one-dimensional CuO chains enhance the b-axis conductivity and contribute little to the Hall conductivity [3], meaning that the measured Hall coefficient, R_H is not equivalent to the planar Hall coefficient (as is generally assumed for structures containing only CuO2 planes). The planar Hall coefficient in YBCO is obtained by multiplying R_H by the in-plane resistivity anisotropy, ρ_a/ρ_b. This ratio is known to be strongly temperature and doping dependent above Tc, but its behaviour as T→0 is less well studied due to the large magnetic fields required to suppress superconductivity. We present new pulsed field measurements (~68 T) of ρ_a/ρ_b and R_H in overdoped YBCO single crystals and discuss changes in the low temperature planar carrier density observed between optimal doping (p=0.16) and p* (p≈0.19).

[1] Badoux et al., Nature 531, 210 (2016)
[2] Putzke et al., Nature Physics, 17, 826 (2019)
[3] Segawa et al., PRB 69, 104521 (2004)

Suppression of back-tunnelling events in hybrid single-electron turnstiles by using AC bias drive

Dr Marco Marín-Suárez[1], **Professor Yuri Pashkin**[2], Dr Joonas Peltonen[1], Professor Jukka Pekola[1]
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Session: Spintronics, July 3, 2024, 14:00 - 16:10

Hybrid turnstiles have proven to generate accurate single-electron currents that underpin electric current metrology. The usual turnstile operation involves setting the working point of the device by adjusting the DC bias and gate voltages, and application of an AC harmonic signal to the gate. This corresponds to the straight pumping trajectory on the bias voltage–gate voltage plane and results in the well-defined current plateaus in the transport characteristics. The accuracy of charge pumping at high operation frequencies is limited, among other errors, by the so-called back-tunnelling events when electrons tunnel in the direction against the applied bias. Increase of the barrier transparency between the island and the leads as well as the source-drain bias suppresses these, but leads to some additional errors. We experimentally demonstrate a driving protocol that suppresses back-tunnelling, thus extending the range of frequencies for generating accurate single-electron currents. The main feature of this approach is an additional AC harmonic signal applied to the bias with frequency twice that applied to the gate electrode. This allows additional modulation of the island chemical potential and improves the single-electron current accuracy by one order of magnitude. We also show that accurate single-electron currents can be generated at zero average bias voltage by applying only AC drive to the bias. Furthermore, we show that within this protocol, the current direction can be reversed by shifting the phase of the source signal. This novel drive method can find applications in quantum sensing and quantum computing.

Nanocalorimetry of CeRh2As2

Mr Maximilian Tobermory Pelly[1], Dr Mari C. Cole[1], Dr Craig V. Topping[1], Prof (apl) Dr Jürgen Weis[2], Dr Thomas Reindl[2], Dr Ulrike Waizmann[2], Dr Seunghyun Khim[3], Dr Andreas W. Rost[1,2]
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Session: Superconductivity 2, July 3, 2024, 14:00 - 16:10

$CeRh_2As_2$is a recently discovered unconventional heavy fermion superconductor displaying two superconducting phases.[1] A suspected quadrupolar density wave transition exists above the superconducting domes.[2] This intersects with them as a function of field leading to speculation that it may be involved in the superconducting transition. Significant broadening and weak signatures of thermodynamic transitions has hindered attempts to fully track the intersection of these transitions, preventing a proper understanding from being gained.[1,3]
We solve this by utilising a newly developed nanocalorimeter based on combination of silicon nitride membranes with primary Coulomb blockade thermometry[4] to enable studying of 100 micron microcrystals of $CeRh_2As_2$. Microcrystals allow greater screening and circumvention of large scale sample inhomogeneities. We observe sharper transitions and higher onset transition temperatures compared to mm sized samples of the same generation, more in line with transition temperatures observed in transport. This has allowed tracking of the QDW all the way to intersection at 6.5 T, well above the SC1 to SC2 transition. We reveal three distinct regimes as a function of field with broad signatures in both normal to superconducting transition jump heights and below Tc field dependent specific heat around the 4 T SC1 to SC2 transition and around 7 T following intersection with the QDW.

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The development of high-Q tantalum superconducting microwave coplanar waveguide resonator arrays

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Session: Polaritons 2 and cavity QED, July 2, 2024, 14:00 - 16:00

α -Tantalum is one of the superconducting materials which has attracted a lot of interest due to its low-loss oxide compared to the other materials and as a result high-quality performance and high relaxation time. Ta can be deposited on a heated sapphire substrate or unheated/heated silicon (Si) substrate with/without a seed layer. Here, we designed, fabricated and measured 40 nm thick α-Ta superconducting microwave coplanar waveguide resonator (CPW) arrays on an unheated Si substrate with an Nb seed layer to promote the growth of α – Ta. After DC measurement for a bare Ta sample, we observed that the Tc of structure is about 4.06 K. After wire-bonding the sample to the copper sample box, mounting it to the dilution refrigerator (DR) and cool-down to the base temperature T=77 mK, frequency spectroscopy measurement showed three resonance frequencies between 3-8 GHz due to three quarter-wavelengths ($\lambda/4$) resonators. Then, power sweep analysis showed that the internal quality factor (Qi) reaches beyond 10^6 at high power for fr= 3.65 GHz. For two other resonance frequencies, the Qi is 9.73 ×10^5 and 8.2 ×10^5, respectively. Two-level system (TLS) loss is the reason for low Qi at low temperatures and power. TLS loss is power and temperature-dependent and has the highest value in low power and temperature and exists in the interface of metal-air, substrate-air and metal-substrate. In this talk, we will discuss the detailed fabrication and measurement of high-Q Superconducting CPW resonators which can be used in different applications such as quantum computing.

Tunable superconductivity in 300 mm CMOS-compatible ZrN nanoconstrictions

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Session: Polaritons 2 and cavity QED, July 2, 2024, 14:00 - 16:00

The phenomenon of gate-controlled superconductivity (GCS) is still under debate but was shown to be fabrication and material dependent [1]. Transferring the fabrication onto CMOS-compatible platforms promises significant integration and scaling potential for quantum control electronics. Compared to conventional CMOS materials exhibiting GCS, such as TiN [2] or Al [3], the properties of ZrN further benefit miniaturization endeavors above 4.2 K [4]. Here, by leveraging the fabrication on state-of-the-art 300 mm semiconductor process equipment, we demonstrate the characteristics of ZrN-based nanoconstrictions displaying the GCS effect.

In initial electrical measurements without applied gate voltage, the constrictions exhibit under- and overdamped switching behavior, depending on size and temperature. The field-dependent critical currents are modulated by Fraunhofer-diffraction like features, effectively demonstrating Josephson current tunneling. By applying ambipolar gate voltages, the critical currents can be tuned down to full suppression. The onset of the suppression is exponential and shows no significant dependence on temperature or magnetic field, implying mainly geometry dependent characteristics. A gate leakage current is exhibited with the occurrence of critical current suppression. This implies electric-field-dependent extraction/emission of high-energy electrons, disturbing superconductivity locally by decay into phonons [2].

The results promise ZrN to be a viable material for the implementation of GCS-based transistors on scalable CMOS-compatible process technology.

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Non-conservation of the valley density and its implications for the observation of the valley Hall effect

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Session: 2D materials 2, July 4, 2024, 14:00 - 16:00

We show that the conservation of the valley density in multi-valley insulators is broken in an unexpected way by the electric field that drives the valley Hall effect. This implies that time-reversal-invariant fully-gapped insulators, in which no bulk or edge state crosses the Fermi level, can support a valley Hall current in the bulk and yet show no valley density accumulation at the edges. Thus, the valley Hall effect cannot be observed in such systems. If the system is not fully gapped then valley density accumulation at the edges is possible. The accumulation has no contribution from undergap states and can be expressed as a Fermi surface average, for which we derive an explicit formula. We demonstrate the theory by calculating the valley density accumulations in an archetypical valley-Hall insulator: a gapped graphene nanoribbon. Surprisingly, we discover that a net valley density polarization is dynamically generated for certain edge terminations. We will draw general conclusions which apply to other phenomena, such as the orbital Hall effect.

Epitaxial growth of large-area monolayers and van der Waals heterostructures of transition-metal chalcogenides

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Session: Thin Films, July 5, 2024, 10:30 - 12:30

Transition-metal chalcogenides (TMC) include some of the most important two-dimensional (2D) materials, hosting unique and disparate electrical, mechanical and optical properties. To gain full control over these properties, it is necessary to combine different chalcogen based compounds in heterostruc-ture 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 for control and practical utilization of the remarkable properties TMC based function-al devices offer. 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 by low coverage, unfavourable morphologies, the premature onset of bilayer formation, and the presence of rotational dis-order. 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 semiconducting materi-als is demonstrated before, it has not been explored for the epitaxial growth of 2D materials. Here, we study the role of sacrificial surfactant species on the growth rate, stabilisation and enhancement of layer-by-layer growth mode, and optimization of carrier lifetimes for various 2D TMCs. Through this, we demonstrate improved crystalline quality and uniform monolayer surface coverage over extended areas and show the first proof-of-principle for exploiting this in the growth of high-quality epitaxial heterostructures of TMCs.

Third-Order Thermoelectric and Spin Photocurrents in 2D Topological Electronic Systems

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Session: Spintronics, July 3, 2024, 14:00 - 16:10

The unique potential of nonlinear photocurrent in probing quantum materials is attracting significant attention [Nat.Rev.Phys 5,170(2023)]. This relies on higher-order correlations, revealing quantum geometry and many-body properties beyond linear response.

Our theoretical studies delve into light-induced third-order currents in 2D electronic systems in WTe2 and Bi2Te3, employing semiclassical and diagrammatic quantum transport theories.

Our investigation into nonlinear spin-photocurrent in WTe2 [1] reveals a nonlinear spin-current for light frequencies within the electronic bandgap. This nonlinear effect is third-order in light field E and is related to the spin-Berry-curvature. This prediction extends our understanding of in-gap photocurrents in the spin-channel, shedding light on third-order responses beyond previously discussed second-order in-gap charge-photocurrents [PRL 125,227401(2020)]. These findings guide future exploration of nonlinear spin-current in THz applications, minimising hot electron effects in the in-gap regime.

I will highlight another third-order current driven by the light field and thermal gradient, termed nonlinear thermoelectric-photocurrent [2]. In 2D Fermi liquids, odd-parity Fermi surface deformations show unusually slow relaxation rates [PRL 123,116601(2019)], suppressed as ~T^4 with temperature T, diverging from the typical Fermi-liquid scaling of ~T^2. We establish a direct relationship between nonlinear thermoelectric-photocurrent and the prolonged relaxation times of odd-parity modes in topological Fermi liquids, characterised by novel topological heat capacitance terms related to Berry curvature. We predict a strong and highly tunable nonlinear thermoelectric effect on the surface of topological insulators, e.g. bismuth telluride (Bi2Te3), offering promise for future experiments.

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Electronic structure of Cr-intercalated NbSe2 epitaxial thin films studied by angle-resolved photoemission spectroscopy

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Session: Thin Films, July 5, 2024, 10:30 - 12:30

In the layered transition metal dichalcogenide (TMDC), intercalation of 3d-transition metal atoms has been widely studied due to the presence of magnetic phases with varied spin-ordering structures. [1] Cr-intercalated niobium diselenide (CrxNbSe2, x: doping amount) is a core example of intercalated TMDC. For $x = 1/3$, the intercalated Cr atoms construct a $\sqrt{3}\times\sqrt{3}$ superlattice, and the system develops a ferromagnetic ordering. On the other hand, when intercalation amount decreases to $x = 1/4$, a 2×2 superlattice develops and the ferromagnetic ordering disappears. [2] Together with magnetic phase changes, strong modulation to the electronic structure has been proposed, including the possibility of intercalated TMDC systems hosting topological phases. [3]

By employing molecular-beam epitaxy (MBE), we obtain well-terminated surfaces while also controlling the intercalated phases of Cr1/4NbSe2 and Cr1/3NbSe2. Angle-resolved photoemission spectroscopy (ARPES) is employed to reveal the electronic structure is modification induced by intercalation. Previously, we have shown the potential signature of the topological band crossing in epitaxially grown ferromagnetic Cr1/3NbSe2 [4]. Here, we examine the temperature-dependent ARPES of Cr1/4NbSe2 thin-films, revealing behavior unique modification at low temperatures. By considering the modification to the magnetic properties of the system, we discuss the electronic structure according to Cr-intercalation amount.

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Evidence for odd-parity superconductivity in $YbRh_2Si_2$, and its enhancement by the onset of electro-nuclear antiferromagnetic order

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Session: Superconductivity 4, July 4, 2024, 14:00 - 16:05

The nature of the interplay between magnetism and superconductivity is a question central to the physics of quantum materials. The heavy-fermion metal $YbRh_2Si_2$ is of particular interest, since it is known to have both antiferromagnetic and ferromagnetic fluctuations.

Here we report a study on single crystals of $YbRh_2Si_2$ by transport and magnetic susceptibility (non-contact probe of complex conductivity), using ultra-sensitive SQUID-based experimental techniques. The results are underpinned by our recent discovery of electronic spin-density wave (SDW) order with onset at $T_A = 1.5$ mK [1].

Superconductivity first manifests below 10 mK. Distinct signatures of superconductivity in the complex sample impedance, broadly reproduced between samples, exhibit different magnetic field dependences, both Pauli-limited and beyond the Pauli limit. This is indicative of odd-parity pairing, and the presence of multiple superconducting order parameters.

Sample-to-sample variations and the absence of corresponding signatures in the heat capacity point towards inhomogeneous superconductivity.

The superconductivity is abruptly boosted on cooling across T_A, suggesting a triplet PDW state. The enhancement is seen both in the kinetic inductance inferred from the transport study, and in the magnetic susceptibility. The transport data also show that the suppression of superconductivity by magnetic field is highly anisotropic, reflecting the underlying electro-nuclear magnetism of $YbRh_2Si_2$.

We find that superconductivity is switched off at the boundary of the primary AFM order. This, together with the enhancement of superconductivity at TA, strongly indicates that magnetic order and fluctuations play the key role in pairing.

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Assessing Nontrivial Topology in Weyl Semimetals by Dichroic Photoemission

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Session: 2D materials 2, July 4, 2024, 14:00 - 16:00

By performing angle-resolved photoemission spectroscopy (ARPES) on the paradigmatic Weyl semimetals Ta(As,P) [1] we show the spectroscopic manifestation of topological features and Weyl physics beyond the simple photointensity over a broad range of excitation energies from the vacuum ultraviolet to the soft X-Ray regime and compare the surface to the bulk band structure [2]. Our experimental observations were complemented by state-of-the-art first principle photoemission calculations based on one-step model of photoemission. The determinant criterion confirms the arc character of the spoon features in the constant energy contour close to Fermi level in non-centrosymmetric TaP. We further show the drawbacks of the existing spectroscopic techniques used to determine whether the given material has non-zero Chern number and discuss an improved approach for identifying Fermi arcs using differential ARPES measurements, their relation to orbital angular momentum (OAM) as well as the proper final state description. Consequently, we conclude that a more realistic description of the final state is needed to explain dichroism by modeling the photoemission matrix element. It immediately follows that the relation between dichroic ARPES and OAM in the initial state cannot be explained within the simplified free-electron (FE) final state picture.

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Conductance asymmetry and current distributions in proximitized magnetic topological insulator junctions with Majorana modes

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Session: Electronic Structure 1, July 3, 2024, 10:30 - 12:40

The chiral topological superconductor, which supports propagating nontrivial edge modes while maintaining a gapped bulk, can be realized hybridizing a quantum-anomalous-Hall thin slab with an ordinary s-wave superconductor. In wide (filmlike) and narrow (wirelike)) geometries such system has been predicted to host chiral Majorana edge states and Majorana bound states, respectively. We theoretically discuss electronic transport via Majorana states in magnetic topological insulator-superconductor junctions with an asymmetric split of the applied bias voltage [1]. We study normal-superconductor-normal (NSN) junctions made of narrow or wide magnetic topological insulator slabs with a central proximitized superconducting sector. The occurrence of charge-nonconserving Andreev processes entails a nonzero conductance related to an electric current flowing to ground from the proximitized sector of the NSN junction. We show that topologically protected Majorana modes require an antisymmetry of this conductance with respect to the point of equally split bias voltage across the junction. When sweeping the voltage bias in filmlike junctions, the pattern of electric currents in the normal leads spans three main regimes [2]. From single-mode edge-current quantization at low bias, to double-mode edge current oscillations at intermediate voltages and up to diffusive bulk currents at larger voltages. Observing such patterns by resolving the spatial distribution of the local current in the thin slab could provide additional evidence, besides the global conductance, on the physics of chiral topological superconductors.

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Theory of Electronic Structure and Optical Properties of Graphene Quantum Dots

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Session: Electronic Structure 1, July 3, 2024, 10:30 - 12:40

Graphene is a material with fascinating transport properties, but with a limited scope for opto-electronic applications because of its gapless nature. One way to overcome this hurdle is to work with nanostructures of graphene nanoribbons or graphene nanodisks many of which are gapped because of their reduced dimensions, and resultant quantum confinement. However, to realize the full potential of graphene nanostructures in optoelectronic applications, it is essential to obtain a deep understanding of their electronic structure and optical properties. In this talk, we will discuss the theory of electronic structure and optical properties of graphene quantum dots (GQDs) within a Pariser-Parr-Pople (PPP) model Hamiltonian-based correlated electron approach, developed in our group. We will present the results of theoretical calculations of the optical absorption spectra of GQDs of different shapes and sizes. The large-scale multi-reference configuration interaction methodology employed in this work ensures that our calculations include electron correlation effects to a high order. We will benchmark our PPP-model calculations against the state-of-the-art time-dependent density-function-theory (TDDFT) calculations.

Investigation of anti-corrosion properties of iron alloys by XPS and Mössbauer Spectroscopy

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Session: New Materials 2, July 2, 2024, 14:00 - 16:00

Corrosion is defined as the chemical or electrochemical reaction between a material, usually a metal or alloy, and its environment that produces a deterioration of the material and its properties. George F. Hays from The World Corrosion Organization estimated that the annual cost of the process worldwide is over 3% of the world's GDP. Therefore, our current study is focused on developing a new class of extremely corrosion resistant iron alloys with very low solutes content using the oxygen-induced surface segregation process.
Our research include preparation of the samples by arc melting or mechanical alloying, heating at ultra-high vacuum (UHV) to induce surface segregation of the solutes and oxidation at high temperatures at the atmospheric conditions. The chemical composition on the surface of investigated sample after heating at UHV was studied by XPS and content of iron oxides after oxidation was determined by Transmission Mössbauer Spectroscopy.

New family of Ti-rich HEA superconductors with high upper critical field

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Session: New Materials 2, July 2, 2024, 14:00 - 16:00

High Entropy Alloys (HEA) are solid solutions of five or more elements mixed in non-negligible proportions (more than 5 at.% of each element). They have recently attracted much attention because of their unique and very promising physical properties. They form well-defined, simple, close packed structures (body centered cubic, face centered cubic or hexagonal). The name HEA comes from the large changes in configurational entropy during the formation of a solid solution from multiple elements. Due to their structural features, HEAs are known for their exceptional mechanical properties, thermal stability, and corrosion resistance. These materials have great potential for various applications if their high durability is combined with more sophisticated phenomena, such as magnetic ordering and superconductivity.

These qualities can make HEA superconductors a good substitute material for brittle Nb-based electromagnets.
Up to now, most of the reported HEA superconductors were based on doped NbTa matrices. Reliable reports are showing that those alloys can exhibit upper critical field in 8-9 T range, which is not high enough to consider them a suitable replacement for materials like Nb-Ti (with upper critical field ~ 15 T, which strongly depends on purity and fabrication method).

We present the first results of synthesis, structural and physical characterization of two new Ti-rich HEA superconductors exhibiting much higher upper critical fields than any NbTa-based HEA previously reported. Apart from theoretical calculations with structural and physical characterization we would also like to present a perspective for research into this family of superconducting HEA.

Electronic Behaviour at Commensurate Interfaces between Semi-Infinite Graphite Crystals

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Session: Electronic Structure 1, July 3, 2024, 10:30 - 12:40

The two common stackings in graphite crystals are Bernal (ABA) and rhombohedral (ABC), distinguished from each other by the relative position of every third layer. The electronic behaviour on the surface of multilayer graphene stacks and semi-infinite graphite crystals of both stacking types has previously been investigated, with localised electronic states known to arise due to rhombohedral stacking faults. Here, we study the electronic properties of the interfaces between infinite crystals of either stacking using Green's functions to derive embedding potentials that capture the influence of layers far away from the interface. We discuss all 13 distinct interfaces which we group into six categories based on the characteristic density of states features in the interfacial region. We also investigate the charge redistribution induced in the vicinity of the interface by the breaking of translational symmetry in the out-of-plane direction. We show that for some interfaces the impact of the latter can lead to on-site energy shifts ~10 meV. These studies provide a foundation for future work on surfaces misaligned by a small twist angle, with the aim to exploit the rich moiré induced physics observed in twisted bilayer graphene in a truly 3D structure.

Fragile dislocation modes

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Session: New Materials 2, July 2, 2024, 14:00 - 16:00

We present the concept of fragile dislocation modes, localized within a specific part of a topological phase while otherwise leaking bulk continuum. As illustrated in this work, these dislocation modes emerge within a confined atomic topological phase in the two-dimensional Su-Schrieffer-Heeger model. Nevertheless, their existence is restricted to a finite region characterized by an indirect gap at high energy. These dislocation modes appear as chiral pairs at specific energies, receiving protection through a combination of chiral (unitary particle-hole) and point group (C4v) symmetries, but only in the presence of an open indirect gap. In this parameter range, we confirm the stability of these defect modes by monitoring their localization and introducing a weak chemical potential disorder explicitly. Consequently, our findings hold significance for the experimental identification of such modes in engineered topological crystals and classical metamaterials.

Charge and heat current fluctuations of quantum Hall edge channels in the heat Coulomb blockade regime

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Session: Non-equlibrium and Quantum Thermodynamics, July 3, 2024, 14:00 - 16:10

Manipulation and detection of heat currents along chiral quantum Hall edge channels connected to a floating Ohmic contact (OC) have recently enabled detailed investigations of quantum heat conduction. These advancements provide opportunities for both fundamental discovery, e.g., the quantisation of ballistic heat conductances, as well as for exploring novel quantum technologies, e.g., small-scale heat-to-work-conversion.

While it is known that the charge current fluctuations emanating from the OC along the edge channels are highly sensitive to the OC electrical capacitance at low temperatures, far less understood are the emitted heat current fluctuations which determine the precision of the heat transport.

In this talk, I describe recent theoretical work filling this gap. By using a combination of bosonization and a Langevin-based approach, I demonstrate how the interplay of the OC electrical capacitance and the OC heat capacity impacts both emitted charge and heat current fluctuations. In particular, I discuss how the generically non-equilibrium aspects of the emitted fluctuations are captured by different measures of effective temperatures. I also show how both charge and heat current fluctuations may be affected by a “teleportation-like” effect of transmitting heat and charge across the OC. These results provide novel opportunities to experimentally investigate and harness the quantum nature of heat in strongly coupled electron circuits.

jeff=1 magnetism and spin-orbit excitations in FeGa2S4

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Session: Magnetism 1, July 2, 2024, 10:30 - 12:40

FeGa2S4 is a two dimensional van der Waals magnet built on a triangular motif of S=2 Fe2+ ions. This compound does not show observable spatially long-range magnetic order and displays analogous thermodynamic transport to S=1 NiGa2S4. We study powders of FeGa2S4 with neutron spectroscopy. We observe multiple excitation bands and parameterize the behavior based on a multi-level spin-orbit exciton model. We argue that typical spin-only descriptions of the magnetism are inadequate and that orbital degrees of freedom are relevant. Based on this, we suggest that FeGa2S4 is rather a jeff=1 magnet making a stronger link to the reported behavior in S=1 NiGa2S4.

Odd-frequency superfluidity from a particle-number-conserving perspective

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Session: Topology, July 2, 2024, 10:30 - 12:30

We investigate [1] odd-in-time—or odd-frequency—pairing of fermions in equilibrium systems within the particle-number-conserving framework of Penrose, Onsager [2] and Yang [3], where superfluid order is defined by macroscopic eigenvalues of reduced density matrices. We show that odd-frequency pair correlations are synonymous with even fermion-exchange symmetry in a time-dependent correlation function that generalises the two-body reduced density matrix. Macroscopic even-under-fermion-exchange pairing order is found to emerge from conventional Penrose-Onsager-Yang condensation in two-body or higher-order reduced density matrices through the symmetry-mixing properties of the Hamiltonian. We identify and characterise a transformer matrix responsible for producing macroscopic even fermion-exchange correlations that coexist with a conventional Cooper-pair condensate. Furthermore, a generator matrix is shown to be responsible for creating macroscopic even fermion-exchange correlations from hidden orders such as a multi-particle condensate. The essential aspects of the transformer scenario can be illustrated using the spin-imbalanced Fermi superfluid as an example. The generator scenario can be demonstrated by the composite-boson condensate arising for itinerant electrons coupled to magnetic excitations. Structural analysis of the transformer and generator matrices is shown to provide general conditions for odd-frequency pairing order to arise in a given system.

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Evidence of folded pseudochiral Fermi surface in the layered charge density wave of 4Hb-TaSe2

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Session: 2D Materials 1, July 3, 2024, 10:30 - 12:40

Due to their multiple possible polytypes, the tantalum dichalcogenides have emerged as a platform to generate clean and controllable material interfaces between metallic, superconducting and putative Mott insulating layers. Here, we report on the electronic structure of 4Hb-TaSe2, a polytype which consists of alternately stacked layers with octahedral “T” and trigonal prismatic “H” coordination of tantalum. The material is known to host a charge density wave (CDW) phase with commensurate formation of 13-atom star clusters in the T-layers, but compared with the much-studied 1T-Ta(S,Se)2, interlayer hopping between clusters is suppressed due to the intercalating metallic H layers. Using selective area angle resolved photoemission spectroscopy (ARPES) combined with ab initio calculations, we unveil that the T surface is metallic, exhibiting a finely structured Fermi surface arising from band folding caused by the star cluster reconstruction. The Fermi surface is further found to be pseudochiral. Theoretical analysis supports the metallic nature of the system and importantly a non-negligible interlayer interaction causing some three-dimensionality to the Fermi surface, and charge transfer between T and H layers. Our new findings will be set in the context of a longstanding debate over the interpretation of previous data from ARPES and other techniques on the 1T-Ta(S,Se)2 which do not show any spectral weight at the Fermi level, and will be further compared to recent high-profile experimental and theoretical works on H-T bilayers.

Unique interplay between magnetic irreversibility and vortex behaviour in the ferromagnetic Fe-based superconductor EuFe2(As1-xPx)2

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Session: Superconductivity 2, July 3, 2024, 14:00 - 16:10

The EuFe2(As1-xPx)2 system features a complex phase diagram characterized by various magnetically-ordered phases. Intriguingly, within the range of approximately 0.15 < x < 0.3, a region of superconductivity emerges, reaching a maximum transition temperature of T_c ~ 25 K at x ~ 0.21. Notably, this superconducting dome overlaps with a ferromagnetic phase that onsets at T_FM ~ 19 K.

Conventionally, ferromagnetism is perceived as antagonistic to singlet superconductivity, given the substantial internal exchange energy that typically exceeds the condensation energy. However, in EuFe2(As1-xPx)2, the spatial separation of the superconducting FeAs layers and magnetically ordered Eu ions within the crystal structure enables the coexistence of these two orders. This unique situation presents an exciting opportunity to investigate the impact of intrinsic magnetic ordering on the superconducting state as the magnetic order is "switched on".

To explore this scenario, we systematically examine the magnetic hysteresis and magnetic relaxation properties of single crystals of EuFe2(As1-xPx)2, encompassing both T_FM < T_c and T_c < T_FM. Our findings indicate that the measured magnetic irreversibility is strongly dependent on the presence of both the magnetic and superconducting orders, and, additionally, the vortex relaxation behaviour is highly sensitive to the onset of magnetic order. Furthermore, complementary magnetic imaging measurements of a sample with T_c > T_FM in zero and applied magnetic field reveal a complex evolution of magnetic structures due to the interplay of the ferromagnetic domain structure and superconducting vortex state. We discuss how these domain structures influence the magnetic relaxation properties of this system.

Topological Textures in Momentum Space and Their Entanglement Properties

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Session: Topology, July 2, 2024, 10:30 - 12:30

We introduce methods of characterizing entanglement, in which entanglement measures are enriched by the matrix representations of operators for observables. These observable operator matrix representations can enrich the partial trace over subsets of a system's degrees of freedom, yielding reduced density matrices useful in computing various measures of entanglement, which also preserve the observable expectation value. We focus here on applying these methods to compute observable-enriched entanglement spectra, unveiling new bulk-boundary correspondences of canonical four-band models for topological skyrmion phases and their connection to simpler forms of bulk-boundary correspondence. Given the fundamental roles entanglement signatures and observables play in study of quantum many body systems, observable-enriched entanglement is broadly applicable to myriad problems of quantum mechanics.

arXiv:2312.09153 [quant-ph]

Sliding induced multiple polarization states in two-dimensional ferroelectrics

Dr. Peng Meng[2,3], **Dr. Yaze Wu**[1], Dr. Renji Bian[2], Mr. Er Pan[2], Dr. Biao Dong[4], Dr. Xiaoxu Zhao[5], Dr. Jiangang Chen[2], Dr. Lishu Wu[6], Dr. Yuqi Sun[2], Dr. Qundong Fu[6], Dr. Qing Liu[2], Dr. Dong Shi[2], Dr. Qi Zhang[4], Prof. Yong-Wei Zhang[1], Prof. Zheng Liu[6,7,8], Prof. Fucai Liu[2,3]

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Session: New Materials 1, July 2, 2024, 10:30 - 12:30

When the atomic layers in a non-centrosymmetric van der Waals structure slide against each other, the interfacial charge transfer results in a reversal of the structure's spontaneous polarization. This phenomenon is known as sliding ferroelectricity and it is markedly different from conventional ferroelectric switching mechanisms relying on ion displacement. Here, we present layer dependence as a new dimension to control sliding ferroelectricity. By fabricating 3R MoS2 of various thicknesses into dual-gate field-effect transistors, we obtain anomalous intermediate polarization states in multilayer (more than bilayer) 3R MoS2. Using results from ab initio density functional theory calculations, we propose a generalized model to describe the ferroelectric switching process in multilayer 3R MoS2 and to explain the formation of these intermediate polarization states. This work reveals the critical roles layer number and interlayer dipole coupling play in sliding ferroelectricity and presents a new strategy for the design of novel sliding ferroelectric devices.

Charge Transport in Molecular Junctions

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Session: Hybrid Organic/Inorganic, July 3, 2024, 10:30 - 12:40

Charge transport in molecular junctions, particularly under strong coupling conditions, poses significant challenges for molecular electronics. Traditional modelling techniques, such as Polaron-transformed Master equations (suitable mainly for weak coupling) and Hierarchical Equations of Motion (optimized for high temperatures), struggle to accurately represent systems strongly coupled to fermionic leads, mainly due to assumptions of minimal system-environment memory effects. This limitation is crucial in device manufacturing, where control over molecule-lead interactions is complex.

Our work harnesses recent advancements in tensor networks and the Automated Compression of Environments (ACE) techniques to address these challenges [1]. ACE employs a framework of tensor networks and matrix product states, which, unlike Markovian master equations, account for the non-Markovian dynamics inherent in strongly coupled systems. This approach integrates influence functions that capture the full memory effects of the environment, allowing for a more precise depiction of the temporal and quantum mechanical complexities of the system-environment interactions.

Preliminary results utilizing ACE illustrate significant deviations from predictions made by traditional weak-coupling master equations, unveiling complex dynamics and interactions previously unaccounted for. Moreover, ACE mitigates the computational burdens typically associated with non-Markovian approaches, providing an efficient and scalable method to explore quantum charge transport phenomena. Our findings not only deepen the understanding of molecular junction dynamics but also pave the way for future explorations into phononic influences on charge transport, thereby enhancing the design and functionality of molecular electronic devices.

1-Cygorek, Moritz, et al. "Simulation of open quantum systems by automated compression of arbitrary environments." Nature Physics 18.6 (2022): 662-668.

Stretch-Induced Tunability of Electrical Transport in 3D Graphene Foam

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Session: Hybrid Organic/Inorganic, July 3, 2024, 10:30 - 12:40

3D graphene foam is widely used in stretchable electronics due to its fast electron transport and mechanical flexibility. In this study, the temperature-dependent electrical resistivity (ρ(T)) of graphene foam is analyzed under various pre-stretching levels. Experimental results demonstrate that ρ(T) changes with increasing pre-stretching levels, indicating a stretch-induced modulation of the electrical transport properties of graphene foam. A conduction network model is proposed to explain the observed ρ(T) by considering the interconnected polycrystalline graphene domains in graphene foam. The model incorporates the thermally activated conduction and phonon-limited conduction within each graphene domain, and the fluctuation-induced tunneling conduction between neighboring domains. By fitting the experimentally obtained ρ(T) into the model, the stretch-induced modulation of the electrical transport of graphene foam is probed by analyzing the alteration in the resistivity of each conduction component. The observed stretch-induced modulation is attributed to the concurrent influence of pre-stretching-induced local strain and conduction network structure change. These findings offer valuable insights into the modulation of electrical transport properties in graphene foam-based stretchable electronics, providing opportunities for further refinement.

Poster Presentations

Competing charge density waves and magnetism in DyTe3

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Poster Session and Drinks Reception, July 2, 2024, 17:30 - 20:30

The rare-earth metal tritellurides are a family of 2D layered quantum materials exhibiting a multitude of correlated electronic phases, including pressure-induced superconductivity, charge density waves (CDWs), and spin density waves (SDWs), enabling the study of how these correlated phases compete and co-exist. DyTe3, one of the heavier compounds in this family, has two competing CDW orders as well as several magnetic phase transitions. The two-dimensional electronic structure of the family lends itself well to surface sensitive techniques such as scanning tunnelling microscopy making it an ideal material to study these phases and their competition by STM.

Here, the interplay of magnetic order and electronic structure in DyTe3 is investigated experimentally using low temperature scanning tunnelling microscopy and theoretically through density functional theory. We present our results that reveal the coexistence of multiple CDW orders and discuss, informed by density functional theory-based calculations, how they impact the electronic structure.

Momentum-dark excitons & trions in InSe with Mexican hat energy dispersion

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Poster Session and Drinks Reception, July 2, 2024, 17:30 - 20:30

We investigate the properties of momentum-dark excitons and trions formed in 2D materials that exhibit a Mexican hat-shaped dispersion relation. In these materials, the electron and hole that couple to create the lowest energy exciton reside at different points in momentum space. These dark excitons therefore have a much-reduced coupling to light and have the potential to have significantly longer lifetimes compared to their bright counterparts.

We focus on monolayer indium selenide which exhibits an inverted Mexican hat-shaped dispersion in the top-most valence band and a parabolic band in the bottom-most conduction band around the Γ-point (Magorrian et al., 2016).

Our calculation reveals the dispersion relation of the momentum-dark exciton in monolayer InSe, which includes information on the activation energy and finite excitonic momentum state. We obtain the ground state binding energy and activation energy via variational techniques based on the 1s- ground state wave function.
Further to this we consider the properties of momentum-dark trions in InSe by including the spin-orbit coupling splitting of the parabolic conduction band.
Beyond this current work, the wider study aims to describe the “brightening” of the dark exciton state through such ways as acoustic phonons (as shown in (Paylaga et al., 2024)) which transfer the required energy and momentum to the dark exciton transferring it to the bright state.
This approach will open new avenues of research such as exploiting dark excitons in solar cells and other semiconductor-based optoelectronic devices.

Discovery of Dynamical Heterogeneity in a Supercooled Magnetic Monopole Fluid

Mr Jahnatta Dasini[1], **Ms Chaia Carroll**[1], Mr Chun - Chih Hsu[2], Mr Hiroto Takahashi[2], Mr Jack Murphy[1], Mr Sudarshan Sharma[4], Ms Catherine Dawson[1], Mr Fabian Jerzembeck[2,3], Mr Stephen J. Blundell[2], Mr Graeme Luke[4], Mr J. C. Séamus Davis[1,2,3,5], Mr Jonathan Ward[1]

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Poster Session and Drinks Reception, July 2, 2024, 17:30 - 20:30

Dynamical heterogeneity, in which transitory local fluctuations occur in the conformation and dynamics of constituent particles, is believed essential for the evolution of supercooled liquids into the glass state. Yet, its microscopic spatiotemporal phenomenology has remained unobservable in virtually all supercooled glass forming liquids. Recent theoretical advances predict that corresponding dynamical heterogeneity should also occur in supercooled magnetic monopole fluids. We searched for the emergence of dynamical heterogeneity when entering the supercooled monopole fluid of Dy2Ti2O7. By measuring the microsecond-resolved spontaneous magnetization noise M(t,T) at temperatures between 14 mK <T <3000 mK we discover a sharp bifurcation in monopole noise characteristics beginning at T≈1500 mK, with the appearance of intense transient fluctuations from powerful monopole current bursts whose magnitude and statistics evolve rapidly with falling temperature. This unique new form of dynamical heterogeneity first emerges upon entering the supercooled monopole fluid regime, reaches a maximum intensity near T≈500 mK and then terminates along with a coincident loss of ergodicity near T≲250 mK. Surprisingly, low intensity monopole noise persists below T≲250 mK, representing activity at approximately 2% of the Dy sites. Its survival to lowest temperatures T≲20 mK reveals a population of quantum dynamical monopoles trapped within the spin-ice ground state. This phenomenology greatly expands our knowledge and understanding of both supercooled monopole fluids and the mysterious ground state of spin-ice.

Magnetic Penetration Depth Measurements of Optimally Doped Yttrium Barium Copper Oxide Crystals Under Hydrostatic Pressure

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Poster Session and Drinks Reception, July 2, 2024, 17:30 - 20:30

Low Temperature Magnetic Penetration Depth measurements are performed on crystals of Yttrium Barium Copper Oxide at a range of pressures between 0 and 3GPa. Optimally doped YBCO crystals are coated on all sides by evaporation with a 300nm layer of lead. The sample is fixed on an inductor coil which is wired to a tunnel diode oscillator circuit whose frequency dependence on the magnetic susceptibility of the circuit acts as a probe for the magnetic penetration depth of the lead-coated sample. The size of the oscillator frequency change at the superconducting transition of the lead coating reveals the magnitude of the Zero-Temperature Magnetic Penetration Depth of the YBCO crystal. The coil is placed in a piston cylinder pressure cell in which hydrostatic pressures of up to 3GPa can be realised. Penetration depth is a quantity that can be related to the density of carriers in a superconductor and their effective mass. Probing this quantity under pressure can provide new insights into superconductor phase diagrams and the presence of quantum critical points. Here, the development of the technique is detailed, along with its use in studying cuprate superconductors.

Valley-polarized Josephson Junctions as gate-tunable 0-π qubit platforms

Yuxuan Deng[1], ZhongChangfei Li[1], Zi-Ting Sun[1], Jin-Xi Hu[1], K. T. Law[1]
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Poster Session and Drinks Reception, July 2, 2024, 17:30 - 20:30

Recently, gate-defined Josephson junctions based on magic-angle twisted bilayer graphene (MATBG) have been fabricated. In such a junction, local electrostatic gating can create two superconducting regions connected by an interaction-driven valley-polarized state as the weak link. Due to the spontaneous time-reversal and inversion symmetry breaking, novel phenomena such as the Josephson diode effect have been observed with zero external magnetic fields. Importantly, when the so-called nonreciprocity efficiency (which measures the sign and strength of the Josephson diode effect) changes sign, the energy-phase relation of the junction is approximate F(ϕ) \propto cos(2ϕ) where F is the free energy and ϕ is the phase difference of the two superconductors. In this work, we show that such a MATBG-based Josephson junction, when shunted by a capacitor, can be used to realize the long-sought-after 0-π qubits which are protected from local perturbation-induced decoherence. Interestingly, by changing the junction parameters to the regime where a large nonreciprocity efficiency is obtainable, transmon-like qubits with large anharmonicity can also be realized. The gate-defined Josephson junctions can be employed as platforms for realizing qubits that are protected from local perturbations.

Optimising nanomagnet arrays for realising topological phases in superconductor-semiconductor quantum devices

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Poster Session and Drinks Reception, July 2, 2024, 17:30 - 20:30

Rotating stray magnetic fields generated by nanomagnet arrays are predicted to induce a synthetic spin-orbit coupling (s-SOC) in hybrid superconductor-semiconductor nanowires commonly used in the search for Majorana bound states [1]. By obviating the need for intrinsic SOC, nanomagnets could thus widen the range of materials available for realising topological superconductivity, for instance to include lower-disorder materials such as carbon nanotubes or silicon nanowires. While recent experiments show that permalloy nanomagnets producing stray fields can shift the energy of sub-gap states in Al/InAs nanowires, generating ~1T local field strengths required to induce a topological phase transition remains a major challenge. The enhanced fields from stacked nanomagnets interleaved with nonmagnetic layers present a potential solution to this problem [2]. In this work we use numerical simulations to explore the intricate dynamics of these arrays. We predict a doubling of the stray field produced by stacking layers of CoFe and investigate the feasibility of integrating these arrays with existing device architectures.

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Directional Superradiance in Chiral Waveguide-Coupled Quantum Dot

Aspen Fenzl[1], Dominic Hallett[1], Luke Hallacy[1], René Dost[1], Luke R. Wilson[1]
[1] *University Of Sheffield, United Kingdom*

Poster Session and Drinks Reception, July 2, 2024, 17:30 - 20:30

The ability to control, predict, and understand the influence of environmental factors on photon-mediated interactions is essential for scalable quantum dot (QD) systems. Despite much theoretical and experimental work on Dicke superradiance, the effects of directional coupling in a waveguide system have yet to be explored fully. To control and alter the behaviour of collective superradiant states [1] has renewed interest in the study of environmental influence on photon-mediated interactions in waveguide coupled systems.

Our work aims to observe directional superradiant behaviour [2] in a broken-symmetry system and study the influence of environmental parameters including pure dephasing, chiral contrast, and relative phase separation. We use an open quantum system approach to understand the role of dissipation and decoherence in an experimental setting. Early simulation results suggest chiral systems reveal features unique to superradiance without the possibility of measurement-induced bunching [3]. This will allow us to unambiguously identify and study superradiant behaviour via Zeeman splitting of individual spin states.

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Magnetic, Transport, and Structural Studies of High-Pressure superconductor La3Ni2O7

Dr Sven Friedemann[1], Dr Dharmalingam Prabhakaran[2], Prof Andrew Boothroyd[2], Prof Simon Hall[1]
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Poster Session and Drinks Reception, July 2, 2024, 17:30 - 20:30

High-temperature superconductivity has been discovered in La3Ni2O7 samples at high pressures [1]. New perspectives on high-temperature superconductivity are now expected from studies of nickelates. It will be important to identify the exact phase responsible for superconductivity. Whilst multiple groups report signatures of superconductivity in resistance and ac susceptibility measurements, some suggest filamentary superconductivity [1–4]. Here, we present DC magnetisation, resistance, and X-ray diffraction measurements on La3Ni2O7. We study samples grown with both the sol-gel method as well as in the optical floating-zone furnace in oxygen pressure and annealed in different conditions. We analyse our results to extract information on the volume fraction of the superconducting state.

[1] Sun, H. et al. Nature 621, 493–498 (2023).
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Towards room-temperature polaritons in a tunable open microcavity using 2D hybrid perovskites

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Poster Session and Drinks Reception, July 2, 2024, 17:30 - 20:30

Quantum optics has seen a tremendous growth in the past few decades. When an exciton in a semiconductor strongly interacts with photons trapped inside the cavity, a new quasi-particle called a polariton is formed. Fine tuning the cavity parameters and exciton energies can alter the interaction strength between them. This strong coupling regime has emerged as an interesting area of research, since it has a variety of applications in quantum information processing and beyond.

To harness the strong coupling between excitons and cavity photons, we sandwich the semiconductor between two mirrors in a Fabry-Perot cavity. Hybrid perovskites are an interesting class of 2D semiconductors that operate at room temperatures. Unlike the conventional 2D materials, perovskites can be easily synthesised in large quantities. Because of their unique multiple quantum well structure, excitons can be confined to individual layers in 2D hybrid perovskites. Thus by altering different parameters of the layers, exciton dynamics can this be changed.

Previous works have demonstrated strong coupling in 2D hybrid perovskites in a FP cavity where both the reflecting mirrors are parallel. At present, we are working with a tunable microcavity that has planar-concave mirrors since this allows better confinement of light. The cavity is also fabricated in a way such that the cavity separation can be altered. Thus, we aim to strongly couple excitons with photons in a planar-concave microcavity and obtain condensates which will be further studied to build a photonic platform that allows quantum optics.

Non-Linear Quantum Optics at a Topological interface

Mr Luke Hallacy[1], Mr Nicholas Martin[1], Dr Mahmoud Jalali Mehrabad[2], Dr Dominic Hallett[1], Mr Xuchao Chen[1], Dr Rene Dost[1], Dr Andrew Foster[1], Dr Luke Brunswick[1], Miss Aspen Fenzl[1], Prof Mark Fox[1], Dr Mohammad Hafezi[2], Prof Maurice Skolnick[1], Prof Luke Wilson[1]

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Poster Session and Drinks Reception, July 2, 2024, 17:30 - 20:30

The integration of topology into photonic devices has the potential to create robust and unidirectional light propagation with strong light-matter interactions [1]. We address the outstanding issues of observing the non-linear effects of single photons in Valley-Hall (VH) waveguides using a novel approach that overcomes issues associated with forming charge traps at etched surfaces and the related spectral wandering of optical transitions [2].

By utilising novel inverse design techniques, it is possible to engineer interfaces capable of efficient mode conversion and topological defect regions for efficient integration of quantum dots (QDs) within a topological photonic environment. We demonstrate the first instances of single-photon resonant fluorescence and resonant transmission spectroscopy of QDs within a topological waveguide. Our results combine topological photonics with optical non-linear effects at the single-photon level, offering a new platform to investigate the interaction between topology and quantum non-linear systems and develop new topological quantum photonic devices [3,4].

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Co-operative and super-radiant emission from electrically-tuneable waveguide-coupled quantum dots

Dominic Hallett[1], Luke Hallacy[1], Julian Wiercinski[2], Rene Dost[1], Nicholas Martin[1], Moritz Cygorek[2], Erik Gauger[2], Maurice Skolnick[1], Luke Wilson[1]

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Poster Session and Drinks Reception, July 2, 2024, 17:30 - 20:30

Coherent interactions between photonic emitters are vital for the scaling up of many quantum information schemes. The fundamental demonstration of interactions between quantum emitters is Dicke super-radiance [1], the formation of an entangled state between the emitters. Waveguide-coupling allows efficient coupling of light between emitters, enabling strong interactions between distant emitters. Recent work has demonstrated the formation of sub- and super-radiant states between two InAs quantum dots (QDs) in a nanophotonic waveguide [2]. In a similar system, it was recently demonstrated that measurements can induce correlations between two emitters that do not interact with each other [3].

This work studies a system of two self-assembled InAs QDs, which are efficiently coupled through a nanophotonic waveguide and independently electrically tuneable. We investigate both super-radiant and co-operative interactions, in the same waveguide-coupled QD system through measurements of the decay rate of the emitters and autocorrelation function of the emitted photons. We observe pronounced quantum beats in the photon statistics, associated with measurement induced cooperativity, that persist with the quantum dots detuned far beyond the dot linewidth. This contrasts strongly with super-radiant emission that requires detuning below the quantum dot linewidth.

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Comparison of superconducting properties of three HEAs with the same valence electron concentration

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Poster Session and Drinks Reception, July 2, 2024, 17:30 - 20:30

Conventional alloys typically consist of one principal element, and one or more dopant elements in small proportion that enhance a certain property of interest. In contrast, high-entropy alloys (HEAs) are composed of multiple principal elements that are all present in major proportion, with the simple structures observed attributed to the high configurational entropy of the random mixing of the elements on their lattice sites [1,2].

In 2014, the first HEA superconductor with the composition Ta0.34Nb0.33Hf0.08Zr0.14Ti0.11 (in at. %) was found [3], revealing a new facet of the capabilities. A variety of studies have been performed on HEA superconductors since that time, aiming to designate their potential for practical applications. In particular, the occurrence of bulk superconductivity in HEAs, which also display excellent specific strength, superior mechanical performance at high temperatures and fracture toughness at cryogenic temperatures, make them promising candidates for superconducting magnets.

This contribution reports on the formation and physical properties of three HEAs Nb0.375Hf0.375Zr0.125Ti0.125, Nb0.375Hf0.125Zr0.375Ti0.125 and Nb0.375Hf0.125Zr0.125Ti0.375. These alloys are composed of the same four elements, have the valence electron concentration (VEC) equal to 4.375 and crystallize in a simple body-centered cubic (bcc) structure. Their superconducting properties were determined by magnetization and specific heat measurements. The discussion compares the obtained results with corresponding data reported for other HEA superconductors.

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Phonon study in Spin-Jahn Teller antiferromagnet: CoTi2O5

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Phonon study in Spin-Jahn Teller antiferromagnet: CoTi2O5
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The Jahn-Teller effect is a phenomenon, where the symmetry spontaneously decreases, affecting orbital and lattice degrees of freedom1. The spin Jahn-Teller effect is observed in pyrochlores, where the lattice of corner-sharing tetrahedra has a large number of spins with the same energy2,3. This issue is resolved by distorting these tetrahedra. Cobalt titanates are of great interest due to their various applications, like catalysis4, microwave devices, and lithium-ion cells. We conducted a neutron spectroscopy study on CoTi2O5, which showed that despite
its lower symmetry compared to pyrochlores and spinels, it still exhibits spin Jahn-Teller driven antiferromagnetism5. This study helps us understand how magnetic interactions work and how spin-phonon coupling can lead to lattice order, as well as identify the right soft phonon modes.
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Extracting Topological Information from Interface Green's Function

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In condensed matter physics, topology is a field concerned with the inherent symmetries of a quantum many-body system unaffected by adiabatic deformations. Topological physics has gained a lot of momentum over the recent years due to the fact that the robust bound states at the boundaries of topological materials have potential applications in quantum information technology. However, it is yet to be seen how we can reliably access the topology of a quantum many-body system in an experiment.

Green's function formalism is a powerful tool for theoretical characterization of quantum many-body systems while being relatively accessible in experiments such as angle-resolved photoemission spectroscopy (ARPES) or scanning tunnelling microscope (STM) measurements. Here, we present an interface Green's function formalism [1], that we have applied to the Su-Schrieffer-Heeger (SSH) model [2]. We have found that the topologically non-trivial phases are closely related to zeros of the inverse interface Green's function.

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Flat Band Josephson Junctions with Quantum Metric

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In this work, we consider superconductor/flat band material/superconductor (S/FB/S) Josephson junctions (JJs) where the flat band material possesses isolated flat bands with exactly zero Fermi velocity. Contrary to conventional S/N/S JJs in which the critical Josephson current vanishes when the Fermi velocity goes to zero, we show here that the critical current in the S/FB/S junction is controlled by the quantum metric length ξ_{QM} of the flat bands. Microscopically, when ξ_{QM} of the flat band is long enough, the interface bound states originally localized at the two S/FB, FB/S interfaces can penetrate deeply into the flat band material and hybridize to form Andreev bound states (ABS). These ABS are able to carry long range and sizable supercurrents. Importantly, ξ_{QM} also controls how far the proximity effect can penetrate into the flat band material. This is in sharp contrast with de Gennes' theory for S/N junctions in which the proximity effect is expected to be zero when the Fermi velocity of the normal metal is zero. We further suggest that the S/FB/S junctions gives rise to a new type of resonant Josephson transistors which can carry sizeable and highly gate-tunable supercurrent.

Quantum Metric induced Ultra-long Crossed Andreev Reflection in Multi-orbital Kitaev Chain

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Poster Session and Drinks Reception, July 2, 2024, 17:30 - 20:30

The study of topological superconductors has been one of the central topics in physics in recent decades due to the possible realisation of Majorana zero energy modes which are non-Abelian particles with potential applications in fault-tolerant quantum computation. While the existence of Majorana modes is known to be protected by nontrivial topology and symmetry of the Bogoliubov-de-Gennes Hamiltonian, the role of quantum metric still remains unrevealed. In this work, we extend the Kitaev chain to a multiband version which supports Majorana zero modes in a nearly flat band with tunable quantum metric and investigate the quantum geometric effects on these Majorana bound states. We point out that both the long-range decay length and the quadratic spread of Majorana wavefunctions are determined by the Brillioun Zone averaged quantum metric. Importantly, with a large quantum metric, the dramatic long-distance decay property helps to sustain the crossed Andreev reflection signal in a much longer device than that of the conventional Kitaev chain. Our study explores the role of quantum metric in topological superconductivity bound states and suggests the possibility for detecting Majorana through crossed Andreev reflection measurements in a significantly long two-terminal device.

Probing electronic properties of quasi-2D metamagnetic materials using Scanning Tunnelling Spectroscopy technique

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Poster Session and Drinks Reception, July 2, 2024, 17:30 - 20:30

Metamagnetic 2D materials have a lot of potential applications in the growing field of spintronics. By the very definition, such systems can provide a sought-after compact magneto-electric interface. Yet, for the majority of discovered compounds, acquired experimental data is insufficient for ab initio modelling of their electronic properties. We use the Scanning Tunnelling Microscope equipped with a high-field vector magnet to resolve the interplay between electronic and magnetic properties in these materials. This report focuses on the van der Waals antiferromagnet TbTe3 [1], which is known to have multiple magnetic transitions at low temperatures under an applied magnetic field [2]. Taking advantage of the Scanning Tunnelling Microscopy's sensitivity to both phenomena, we aim to construct the most comprehensive picture of underlying highly correlated electron physics in this metamagnetic system.

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Spiral Spin Liquid Noise

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No state of matter can be defined categorically by what it is not; yet spin liquids are often conjectured to exist based on the nonexistence of magnetic order. A promising new concept designed to circumvent this ambiguity is to categorically identify each spin liquid type by using its spectrum of spontaneous spin noise.
Here we introduce such a spectroscopy for spin liquid studies by considering Ca10Cr7 O28. This is a spin liquid without magnetic order to below 20mK, but whether classical or quantum and in which specific state, are unknown. Now, using SQUID-based spectrometers, we measure the time and temperature dependence of spontaneous flux and thus magnetization of Ca10Cr7O28 samples. The resulting power spectral density of magnetization noise along with its correlation function, reveal intense spin fluctuations spanning frequencies 0.1 Hz to 50 kHz.
When compared to Monte Carlo simulations for a 2D spiral spin liquid state parameterized for Ca10Cr7O28, comprehensive quantitative correspondence with the data including, and magnetization variance clearly fingerprint the state of Ca10Cr7O28 as a spiral spin liquid.

Superconductivity in UNbTiVZr, a new high entropy alloy containing uranium

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High entropy alloys are materials composed of multiple elements with atomic content between 5% and 35%. These alloys are characterized by properties significantly different from the averaged properties of the constituent elements (this is known as "cocktail effect"). In addition, due to the high configurational entropy resulting from the random arrangement of atoms, these alloys crystallize in simple crystal structures [1, 2] and exhibit exceptional mechanical properties.
Superconductivity in high entropy alloys was discovered in 2014 with the alloy $Ta_{0.34}Nb_{0.33}Hf_{0.08}Zr_{0.14}Ti_{0.11}$ [3]. The combination of good critical parameters and mechanical properties of this type of systems suggests that high entropy alloys may be an attractive alternative to the materials currently used in the production of superconducting magnets.
Since then, many high entropy superconducting alloys have been discovered, but only a few of them contain actinides.
This work presents the superconducting properties of a novel UNbTiVZr alloy determined from measurements of magnetic properties, specific heat and electrical resistivity. This alloy exhibits type II superconductivity with a critical temperature of 2.1 K and an upper critical field of 5.1 T.

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Spin-induced strongly correlated magnetodielectricity, magnetostriction effect and spin-phonon coupling in helical magnet Fe3(PO4)O3

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Poster Session and Drinks Reception, July 2, 2024, 17:30 - 20:30

The demand for advanced spintronics devices has spurred research into multifunctional materials responsive to various external stimuli. Focus has been on discovering new multiferroic and magnetodielectric materials for various real-world applications. However, such materials are scarce due to the antagonistic origins of their magnetic and electric properties, often limited by low critical temperatures (<40 K). Tailoring materials with higher critical temperatures remains a challenge, with only a few compounds like CuO (Tc ~ 230 K) and certain hexaferrites displaying coupled properties at considerably high temperatures. On the other hand, Spin-phonon coupling (SPC) is a captivating phenomenon in strongly correlated systems, where magnetic and structural phase transformations are reflected in phonon spectra. SPC serves as a gauge for monitoring various exotic properties such as magnetoelectric coupling, spin Seebeck effect, magnetostriction effect, phonon Hall effect, spin-Peierls transition, and thermal Hall effect in multiferroics.
In this report, we demonstrate a spectrum of simultaneously occurring and highly-entangled intriguing phenomena induced by helical spin ordering in a polar and spin-frustrated magnetic system Fe3(PO4)O3. Such phenomena include magnetodielectric coupling with a weak ferroelectric ordering, clear magnetostriction effect manifested as a dramatic down-turn in the thermal variation of lattice parameters, and strong spin-phonon coupling (which displays a unique anomalous hardening and softening of various phonon modes) at temperatures as high as TN = 163 K. The observed dielectric peak is seemingly associated to a structural distortion via the strong magnetostriction effect.

Local distortions of the crystal structure in a new High-Entropy Alloys Ti0.5(ZrNbTaHf)0.5 and Ti0.5(VNbTaHf)0.5: DFT study

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Poster Session and Drinks Reception, July 2, 2024, 17:30 - 20:30

Superconducting high-entropy alloys (HEAs) are the new category of disordered superconductors. They have been researched since the discovery of superconductivity in Ta0.34Nb0.33Hf0.08Zr0.14Ti0.11 by Koželj et al. in 2014. These materials exhibit exceptional mechanical properties, great stability in extreme temperatures, and significant robustness to high pressure. Such properties make them a perfect candidate for high-field magnets in LHC, ITER, or NMR applications [1].
HEAs are solid solutions of five or more elements, each with a concentration between 5 and 35 at. %. They have high configurational entropy, and because of that – high chemical and structural disorder [2]. In this work, four type-A HEA superconductors: Ti45.0Zr13.1Nb14.8Ta13.6Hf12.5, Ti47.9Zr13.8Nb14.1Ta11.4Hf12.6, Ti47.0V11.8Nb14.8Ta14.5Hf11.5, Ti49.6V13.1Nb13.3Ta10.7Hf13.3, were investigated within density functional theory (DFT). Theoretical studies were performed using two well-suited approaches for disordered systems: the Korringa-Kohn-Rostoker method with coherent potential approximation (KKR-CPA) and projector augmented wave (PAW). In the second method, twelve special quasi-random structures (SQS) were generated, with three atomic configurations for each HEA system. Not only static calculations were performed, but relaxation of crystal structure was also considered. The formation of local distortions and their influence on electronic structure, electron-phonon interaction, and superconductivity were explored and compared to experimental data.

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Superconductivity in Ca intercalated bilayer silicene

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Superconducting quantum materials are becoming indispensable components for quantum devices, encompassing various applications, ranging from quantum computers to power transmission systems. This manuscript employs density functional theory to explore the superconductivity in two-dimensional (2D) calcium (Ca) intercalated bi-layer silicene compound, Si_2CaSi_2, which has been experimentally synthesized. Our findings demonstrate that this system can superconduct below 5.4K, owing to strong hybridization of Ca-3d and Si-3pz bands. The resulting flower-like Fermi surface couples with lower frequency Si and Ca out-of-plane vibrations, which enhance the electron-phonon coupling, as is evident from the large peaks in Eliashberg's spectral function. The superconducting transition temperature (Tc) is comparable with that of experimentally reported Li-decorated monolayer graphene and higher than the Ca-intercalated bilayer graphene systems. The observation of superconductivity in Si_2CaSi_2 places it in the category of covalent superconductors, joining compounds like MgB_2, doped diamond, doped Si, and graphitic intercalated compounds (GIC), which maintain strong covalent bonds in their metallic state. The Tc can be further enhanced by the application of pressure that can flatten the bands near the Fermi energy and enhance the occupancy of the interlayer bands. The incorporation of spin-orbit coupling, which is prevalent in such noncentrosymmetric systems, can further increase the Tc. Our study demonstrates ways of inducing superconductivity in silicon-based 2D systems that can be easily integrated with the existing silicon technology and can revolutionize futuristic device applications.

Catalogue of Non-Fermi Liquid Exchange Models for Doublet Impurities in a Cubic Field

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Poster Session and Drinks Reception, July 2, 2024, 17:30 - 20:30

We examine all possible Kondo type of non-Fermi liquid (NFL) exchange interactions between a doublet impurity and local conduction electrons in a cubic field. First we study the possible couplings between a non-Kramers doublet impurity and surrounding conduction electrons and determine the parameter regions in which two-channel Kondo (2CK) behaviour emerges. We find that the space of couplings is divided into 2CK and one-channel Kondo regions, and that 2CK behaviour is not guaranteed. We also consider all possible exchange interactions between a Kramers doublet impurity and surrounding conduction electrons, which transform as irreducible representations of the cubic point group, and analyse the two resulting NFL quantum impurity models: the topological Kondo model and the spin-half impurity spin-three-half conduction electron Kondo model using the numerical renormalization group (NRG). We derive the thermodynamics of the topological Kondo model using NRG. We also construct a non-spherically symmetric exchange coupling that only has cubic symmetry, and show that it still leads to the same fixed point as the spin-half impurity spin-three-half conduction electron Kondo model. We propose candidate materials where the resulting NFL behaviour could be observed.

Theoretical insight into terahertz spectroscopy of the dye atacamite

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Theoretical insight into terahertz spectroscopy of the dye atacamite
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Atacamite is relatively well known for being formed on the surface of bronze statue due to corrosion. It has 4 polymorphs. The Cu2Cl(OH)3 are grouped as natural cuprates. In the meaning that they contain copper and oxygen, they are like the well-known high-Tc superconducting cuprates where the magnetic interaction between the Cu2+ spins is an essential factor in the occurrence of the high-Tc superconductivity. Therefore we think it is of interest to investigate the behaviors of the Cu2+ spin behaviors in the natural cuprates. First, we investigated the most known compound atacamite. Few papers have been published on the vibrational spectroscopy of these minerals. This may be because many of the bands relating to the CuCl and CuO vibrations occur below 400 cm−1 and are therefore not easily measured. Further techniques such as infrared reKlectance spectroscopy are also limited by cut-off at even higher wavenumbers. Raman spectroscopy has been used to probe the molecular structure of atacamite and paratacamite. only in the last decade Kirst principles calculations for the condensed matter have been published precisely since phononic calculations have become routine. We want to obtain phonons using the ph.x program from the QUANTUM ESPRESSO suite.

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Applying the Bethe-Salpeter equation to muon spin rotation experiments: Opportunities and Challenges

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Over the last decade, density functional theory (DFT) calculations have had a huge impact on the muon spin rotation (μSR) technique, allowing for a fully quantitative analysis of the data from experiments which was simply not possible before. Despite this, DFT calculations suffer from the infamous 'band gap problem', where they tend to underestimate the band gap in various systems which provides a limitation to the application of these calculations to excited muon experiments. Recent state-of-the-art developments in many-body perturbation theory has overcome this problem by applying the Bethe-Salpeter equation to ground state electronic structure calculations, predicting the band gap of various systems to a very high accuracy. In this poster, we report the results of a recent STFC-funded feasibility study of applying such methods to DFT calculations on systems involving an implanted muon, and discuss how such calculations can be utilised to improve μSR experiments, particularly those which involve photo-excitation.

Poster Presentations

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