Understanding the Complex Magnetic Effects in a Low-Dimensional Frustrated Magnet Through Experimental and Theoretical Techniques

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Exotic quantum states such as spin-liquid, spin-ice, and spin-glass phases [1,2,3] have been revealed through investigations of frustrated and quantum magnetic systems, intensifying recent interest in such systems. The natural mineral atacamite, $Cu_2Cl(OH)_3$, represents a low-dimensional quantum frustrated magnet [4] with similarity to spin-liquid systems. Atacamite has a complex magnetic phase diagram [5], however, the transitional dynamics and the spin-structures of its various magnetic phases are not yet completely understood. Many experimental techniques can be applied to characterise the complex magnetic properties of a magnetic system. Magnetisation, susceptibility, specific heat, neutron diffraction, inelastic neutron scattering, and terahertz (THz) spectroscopy have all been applied to atacamite with the goal of describing its magnetic properties and phases.

This work gives a comprehensive overview of both the experimental and theoretical techniques used to determine the magnetic exchange structure of atacamite, with a focus on the experimental techniques of inelastic neutron scattering and THz spectroscopy.

Theoretical density functional theory (DFT) modelling has been performed to calculate the exchange interactions in atacamite. However, empirical results are needed to validate these calculations. Thus, several candidate exchange structure models have been developed from the DFT calculations, and tested against inelastic neutron scattering measurements of atacamite's spin-waves through linear spin-wave theory, revealing a promising exchange structure.

Despite the recent curiosity in atacamite, little is known about its optical spectra in the THz energy region, which corresponds to where magnetic spin-wave modes are often observed in magnetic systems [6,7]. Recent THz measurements have attempted to reveal spin-wave modes, however, evidence for structural phase transitions was found in the spectral temperature dependence of atacamite, highlighting the complex dynamics of the system.

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Electronic Structure of Titania Surfaces Modified by Metal Clusters

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Metal clusters with a size of less than 100 atoms are suitable for modifying the electronic properties of semiconductor surfaces. [1, 2, 3] Metal clusters have been shown to be promising candidates as co-catalysts for photocatalytic water splitting.[4] However, using such clusters as co-catalysts requires implementing processes which suppress their agglomeration on catalyst surfaces. In order to avoid agglomeration of the metal clusters and in order to retain their specific electronic structures, the coverage of the surface with metal clusters has to be kept below 10%. The main challenges in this field are a) to maintain the size and thus the properties of the metal clusters and b) to determine the electronic structure of the clusters.

The first challenge described above is considered as one of the main challenges in the field of surface modification with metal clusters can be addressed by introducing defects on the metal oxide surface, specifically oxygen vacancies. The second challenge can be addressed by using experimental techniques which are exclusively sensitive for the electronic structure of the outermost layer. Metastable Induced Electron Spectroscopy (MIES) is such a technique and has been used successfully to determine the change in electronic structure due to the deposition of Au and Ru clusters. Applying techniques such as singular value decomposition, the changes of the electronic structure can even be quantified. [2]

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Giant *ZT* in topological insulator ultrathin films

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We develop an *ab initio* method to realistically calculate thermoelectric properties of topological insulators based on a combination of first-principles band-structure calculations and semiclassical Boltzmann transport theory. As two examples, we consider thin films of time-reversal topological insulator $Bi_{0.833}Sb_{0.167}$ and crystalline topological insulator $Pb_{0.92}Sn_{0.08}Se$. We find that topologically non-trivial surface states of these topological insulators significantly contribute to the thermoelectric figure of merit *ZT*. The highest *ZT* is achieved for ultrathin films of ~1 nm thickness, as in this case the contribution of the topological surface states to the thermoelectric transport is maximized. Moreover, for ultrathin films of ~1 nm the surface subgap opens at the Dirac point due to hybridization of the surface wavefunctions, and it leads to a much larger Seebeck coefficient. We show that *ZT* as high as 10 can be reached for crystalline topological insulator $Pb_{0.92}Sn_{0.08}Se$ at 120 K. Our *ab initio* approach for calculating realistic values of *ZT* may stimulate a major step forward on the route in using topological insulators as enhanced thermoelectric materials.

ADS-1 and ADS-2: New high-energy X-ray beamlines for advanced materials characterization at the Australian Synchrotron

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The Australian Synchrotron's suite of research beamlines is expanding, with the BRIGHT Project set to deliver eight new operational beamlines at the facility by 2025. Included among these are the two Advanced Diffraction and Scattering beamlines, ADS-1 and ADS-2, which will offer high-energy X-rays (45–150 keV) for a wide variety of diffraction, imaging and tomography experiments. The ADS beamlines will cater to diverse condensed-matter materials and engineering sample types, including powders, single crystals, monolithic solids and functioning devices. The high-energy monochromatic or broad-spectrum ("white") X-ray beams available at ADS will be particularly well-suited to penetrating bulky or strongly-absorbing samples and sample environments, as well as facilitating characterization experiments that require very high momentum transfer (Q) coverage, such as pair distribution function (PDF) analysis to study short-range order in complex materials.

Most major components of the ADS beamlines are currently under construction, with the first user experiments expected to be scheduled in mid-2024. I will present an update on the progress of the ADS project, including the latest design features of the two experimental endstations and the planned range of experimental capabilities.

Using Low Energy Ion Beams to Pattern the Surface of Topological Insulators

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A wide range of ion energies (KeV- MeV), ion species, and ion fluences are achievable by ion beam implantation, which allows fabrication of highly customized patterned subsurface structures in materials. This advanced material processing technology allows tuning of specific magnetic, and electronic properties with the aim of achieving a wide range of functionalities in electronics. Magnetic ions implantation has been actively used for functionalising topological materials in recent few years in attempt to fabricate magnetic topological insulators for spintronic applications.[1, 2] Ion beam patterning, like electron-beam lithography, able to fabricate customised geometryies on a surface of a topological insulators to create a functionalised region with desired electronic and magnetic properties, as illustrated in figure 1. We demonstrate that the current method has the potential application in the integrated circuitry processing industry with the ability to "write" very small features down to few tens of nanometers.

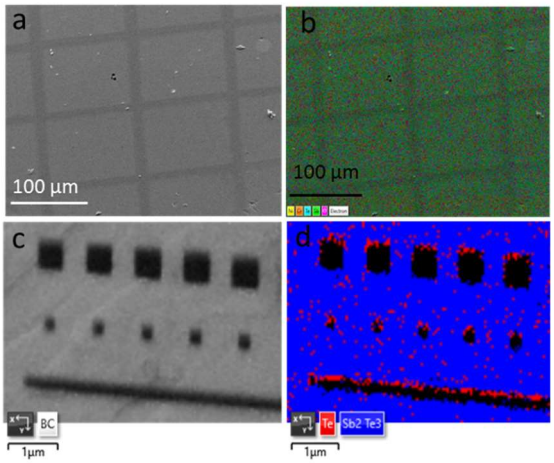

Figure 1. Low energy ion beam patterning of Sb_2Te_3 surface (a) SE image of Sb2Te3 surface patterned with magnetic Cr ions, and (b) corresponding EDS mapping. (c) Band contrast image shows Ga ion beam patterned region on the surface of crystalline Sb_2Te_3 (indexed as dark patterns), and (d) Phase colour identification from electron backscatter mapping.

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A reverse Monte Carlo algorithm to simulate 2-dimensional small-angle scattering intensities

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Small-angle neutron scattering (SANS) and small-angle X-ray scattering (SAXS) are important, experimental techniques for studying the behaviour and properties of materials on the nanoscale. Small-angle scattering (SAS) has been used to investigate systems relevant to a range of scientific fields, including polymers [2], inorganic nanoparticles [3] and magnetic vortices [4]. While the technique is well-established for its versatility and compatibility with a range of sample environments for in-situ studies, analysis of experimentally acquired data is still challenging, particularly in light of the growing complexity of the studied systems.

Numerous out-of-the-box options exist for analysing structures measured by SAS, but many of these are underpinned by assumptions about the underlying interactions that are not always relevant for a given system. In this presentation, we describe a numerical algorithm based on reverse Monte Carlo simulations to model the intensity observed on a SAS detector as a function of the scattering vector. The model simulates a two-dimensional detector image, accounting for magnetic scattering, instrument resolution, particle polydispersity and particle collisions, while making no further assumptions about the underlying particle interactions.

By simulating a 2-D image that can be potentially anisotropic, the algorithm is particularly useful for studying systems driven by anisotropic interactions. The final output of the algorithm is a relative particle distribution, allowing visualisation of particle structures that form over long-range length-scales (i.e., several hundred nanometres), along with an orientational distribution of magnetic moments. We show the effectiveness of the algorithm by modelling a SAS experimental dataset studying finite-length chains consisting of magnetic nanoparticles, which assembled in the presence of a strong magnetic field due to dipole interactions [4].

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Triplons in quasi-1D antiferromagnets

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Spinons and triplons are emergent quasiparticles that are found in quasi-1D antiferromagnets that arise from the collective excitations of localized spin-1/2 objects. As observed in inelastic neutron scattering (INS) and magnetic Raman spectroscopy (MRS), there is evidence that they may determine the low-energy physics of some frustrated two-dimensional antiferromagnets and weakly coupled antiferromagnetic spin chains. The spinon is a mobile, charge neutral, spin-1/2 excitation that is responsible for the large continuum found in INS and potentially those seen in MRS. Triplons occur from the binding of two spinons, and they are fundamentally different from the well-known magnons that are found in ordered magnetic systems. Very little is known about these triplons, and since they are responsible for many important features found in INS and Raman spectroscopy in some quasi-1D antiferromagnets, it is imperative that they are further studied.

We characterize the triplons in quasi-1D antiferromagnets, calculated using perturbation theory of a single chain where the physics is exactly given by the Bethe ansatz. We find that the so called bound and anti-bound triplons both possess density-density spinon correlations that obey a power law at large wavelengths. Using the real-space probability distribution of the triplons, we find that the triplons can be understood as an on-chain localization of the constituent spinon excitations that have similar crystal momentum.

Structural and Magnetic Properties of Platinum and Osmium Vacancy Ordered Double Perovskites

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The structures and magnetic properties of the vacancy double ordered perovskite structures of the form A_2BX_6 (A = Na, K, Rb, Cs; B = Pt, Os; X = Cl, Br, I) are studied (some of which have varying states of hydration). Na_2BCl_6, Na_2BBr_6, K_2BCl_6 and Na_2BBr_6 all undergo two structural phase transitions owing to the states of hydration and temperature; a behavior that is consistent with iridium [1]. Osmium proceeds through a different dihydrate structure than the iridium and platinum isostructural analogues, addressed in this study are the potential causes for this difference. Structure of the platinum complexes (inclusive of changes in hydration) state have been determined for the first time using in-situ variable temperature x-ray diffraction and magnetic properties determined using vibrating-sample magnetometer measurements with a range between 400 - 2K. Magnetic response at low temperatures for some materials indicate weakly magnetic ground states which are inconsistent with the expected $J_{eff} = 0$ ground state.

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On-surface synthesis of 2D organometallic Ag-biphenyl networks

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Two dimensional organometallic (OM) Ag-biphenyl networks were synthesized by the assembly of the tetrapod precursor 3,3',5,5'-tetrabromo-biphenyl on the high symmetry Ag(111) surface. After deposition of the twisted precursor onto a room temperature Ag(111) surface two Br atoms are lost and chain structures are formed, which have been observed previously [1]. Annealing of the surface at 200-250 °C initiates an Ullmann coupling reaction resulting in the loss of the remaining Br atoms and the self-assembly of biphenyl molecules and Ag adatoms into a planar, 2D OM, Ag-biphenyl network. The network consists of two distinct polymorphs: 'brickwall' and 'flower' which exist together in combined domains (Fig. 1). Electronic band structures for the freestanding 2D OM networks of both polymorphs were calculated using Density Functional Theory. The band structure of the 2D brickwall network shows a semimetal character with a Dirac point at the Fermi level along a high symmetry path in the Brillouin zone. The band structure of the 2D flower network in contrast has a band gap at the gamma point of approximately 0.3 eV. Further work will investigate if it is possible to control the domain growth conditions to favor one polymorph over the other.

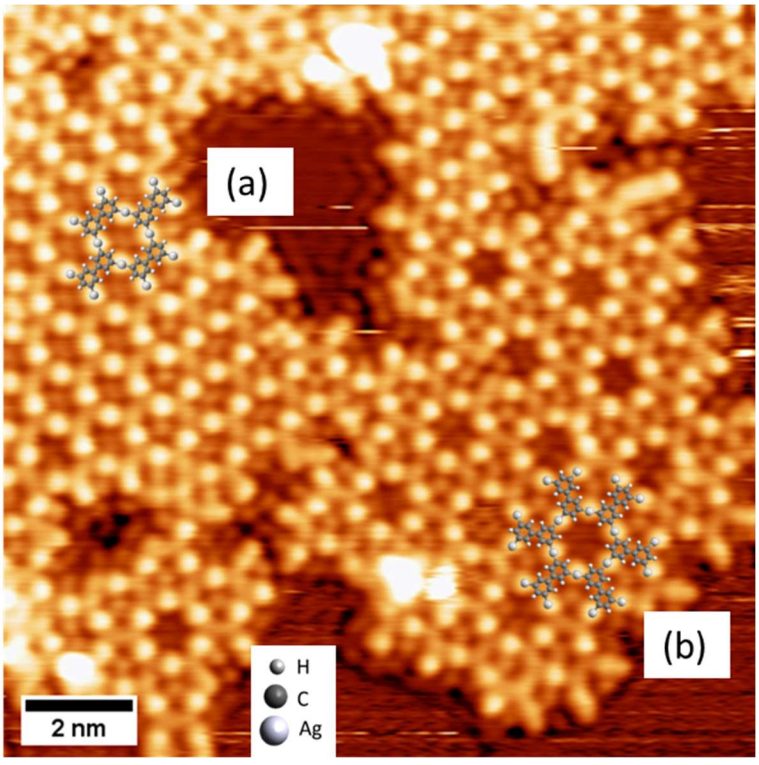

Figure 1. STM image of an OM Ag-biphenyl 2D network on Ag(111) indicating two distinct polymorph structures: *brickwall (a)* and *flower (b)*. 14 nm × 14 nm, V_B = -0.5 V; I_T = 20 pA.

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Magnetism, redox behavior and mixed ionic electronic conductivity in oxygen deficient ferrite perovskites

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The $Ba_3LnFe_2O_{7.5}$ family of compounds are oxygen-deficient perovskites which adopt structures that consist of ordered arrays of corner-linked LnO_6 octahedra and FeO_4 tetrahedra on the perovskite B-sites.[1, 2] Reports of magnetic properties of these compounds have been mixed. The initial study of $Ba_3YFe_2O_{7.5}$ found no evidence of long-range magnetic order down to 5 K, however subsequent studies have found these compounds do show low-temperature magnetic order [1, 2]. The $Ba_3LnFe_2O_{7.5}$ family therefore present a good opportunity to study complex magnetic interactions between magnetic Ln^{3+} 4*f* and Fe^{3+} 3*d* cations. We have made the Y and Dy compositions with this structure and observe long-range antiferromagnetic order at T_N = 6 and 14 K respectively. The Dy composition also shows evidence for metamagnetism with field dependant hysteresis observed below T_N. *Ab initio* density functional theory (DFT) calculations have been used to support the experimental data, e.g. comparing magnetic energies.

Additionally at high temperatures (above 500 K) we have found these materials undergo multiple redox associated phase transitions and show high mixed ionic-electronic conductivity. We have performed variable temperature *in-situ* synchrotron X-ray diffraction experiments; to investigate the crystallographic phase transitions. At approximately 500-600 K depending on Ln cation $Ba_3LnFe_2O_{7.5}$ compounds undergo a first-order phase transition to an orthorhombic phase. The phase transition is correlated with an uptake of O_2 into vacancies in the lattice, accompanied by the partial redox of Fe^{3+} to Fe^{4+}. Impedance spectroscopy measurements show that these phases also have high total conductivities, making them very promising as mixed oxide ion and electronic conductors. DFT including the magnetic structure also provides a much more accurate calculated density of states (DOS) of these materials to understand the associated electronic structure and conductivity.

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Visualizing temperature in MRI to Guide Thermal Cancer Treatments

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The current treatments of cancerous tumors, typically chemotherapy or surgical extraction, are invasive and have significant side-effects. Recently new, less invasive, approaches guided by magnetic resonance imaging (MRI), involving localized heating or freezing have become more prevalent. Temperature measurements are critical for this, however current techniques, typically the proton resonance frequency (PRF) shift, are not always sufficient.

Here we present recent work on developing new techniques that are more robust. We showcase two methods:
1) Temperature measurements which change the intensity of the MR image through the introduction of magnetic nanoparticles or micron sized particles [1]
2) Temperature measurements which change the intensity of the MRI image through the use of soft silicone materials.[2] This technique is particularly important for cryo-surgeries, as the PRF method fails completely below freezing.

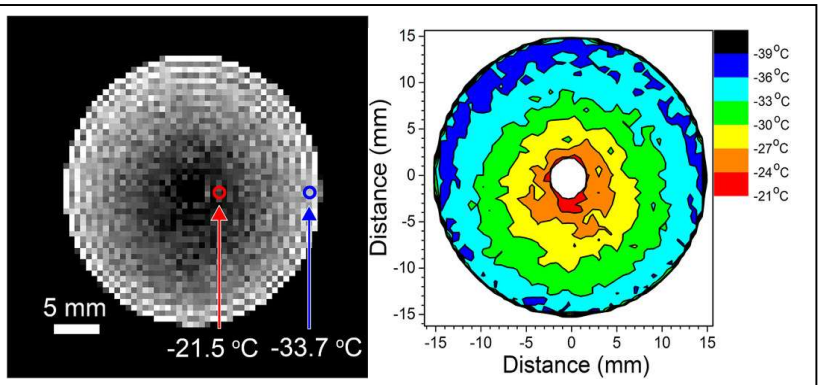

Fig. 1 Direct (T1 weighted) and false color images of sub-zero MRI measurements of a silicone phantom with a temperature gradient between the inner and outer region. The outer region is colder.

The first method involves the development of magnetic particles with a Curie temperature near that of body temperature. These particles create a temperature-dependent inhomogeneous magnetic field which results in a temperature dependent MRI intensity. The second method uses the temperature dependent T1 relaxation times of CH_3 molecules in silicones to change the intensity of the image as in Fig. 1. We discuss how these effects can be implements in clinical settings to obtain temperature information. [3]

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[3] Research partially supported by National Science Foundation grant (SBIR-1843616) and R.E.C. work was also partially supported by the Australian-American Fulbright Commission. Its contents are solely the responsibility of the author.

Analysis of 13th Century Crowdundle Beck Bloomery by Mössbauer and Raman Spectroscopies and SEM

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The bloomery is situated on land granted to William de Stuteville by King John in 1201. It was reported in 1579 that subsequent owners "had digged and gotten leade ore and iron". The land was fought over by the Scots and English and an iron mine capable of producing implements of war would have been prized. This particular furnace appears to have been <1 metre in diameter, with each successive firing being placed directly on top of the previous firing using a grass tempered clay base. Part of the furnace wall was destroyed after each firing to remove the bloom iron produced. No residual iron-containing raw material has yet been found in the survey and the likely form of raw material may have been goethite from an iron deposit higher up Crowdundle Beck or hematite from a little further away. It is probable that alder was used as the timber source for charcoal production.

The bloomery was rediscovered by Barbara Blenkinship in the early 1970's and samples were collected of the charcoal, clay base, slag, slag + bloom and bloom. Radiocarbon dating of the charcoal by Beta Analytical Inc., Miami, Florida, USA placed it at 1295-1410 CE, putting to rest the possibility that it was of Roman origin since they were known to have mined in the area. Mössbauer spectra of the samples showed that only two contained magnetically ordered iron, the lightly fired clay and the bloom, both of which contained magnetite with some hematite in the clay. Both spectra were very complex, with the sextets having magnetic relaxation, and with several doublets as well. The spectra of all the other samples were simple quadrupole split doublets, although the linewidths varied considerably due to the range of chemical concentrations in the samples.

The dominant doublet in most of the spectra was due to the ferrous silicate fayalite, Fe_2SiO_4, which is the iron-rich end of the olivine series. Some of the other doublets are yet to be positively identified with one broad doublet in the clay sample being fitted with a histogram of 13 doublets, which have an interesting curved correlation between the isomer shift and the quadrupole splitting. The maximum quadrupole splitting in the distribution appears to be larger than any ferric quadrupole splitting values in the literature. It is also interesting to note that the Raman spectra pick up many more iron compounds, including goethite and wustite in the slag sample than the Mössbauer spectra have identified.

This research is providing an understanding of the metalworking conducted at this early iron-working site. Time is pressing for a further survey because the nearby river recently flooded the site and washed away much valuable evidence.

To flip or not to flip? Performance and recent results of the spin-polarisation system on the neutron reflectometer at ANSTO

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The surface reflection of X-rays and neutrons can be used to study ultra-thin film structures down to the sub-nanometer scale. Spin polarised neutrons allow for the in-plane magnetic depth profile and vector direction to be determined in films and at crystal surfaces. This poster presents recent spin-polarised neutron reflectometry results from the PLATYPUS reflectometer at the Australian Nuclear Science Technology Organisation. It includes recent determinations of the spin polarisation and flipping ratios for neutrons with wavelengths between 2.5-12 Å and introduces a Python-based software package that has been developed to process the data, correct polarization leakage and solve the 1D Schrödinger equation to quantitatively fit the data. An interactive app is also under development to help new users to learn to align samples and operate the instrument. Finally, some recent applications will be highlighted in ultra-thin 2D magnets [1], strongly correlated oxide films [2], ion-beam irradiated semiconductors [3] and forthcoming work on magnetic topological insulators.

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Intermetallic Compounds in the Gold-Sodium System

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The formation and stability of intermetallic compounds in the atmospheric pressure Au-Na system were studied. The compounds Au_2Na and $AuNa_2$ were readily prepared but obtaining samples containing a phase or phases lying between these two was more difficult. A very diverse range of synthesis techniques was attempted. Investigation is challenging on account of the high reactivity, low melting point, and high volatility of the Na. There was no evidence for AuNa or the AuNa $\rightarrow$ L+Au_2Na reaction at 372 °C that had been reported by earlier workers. Diffraction studies on samples with x_{Na} in the 0.5 to 0.6 range showed Au_2Na and a new phase with peak positions consistent with the Au_2Na_3 predicted by density functional theory (DFT) calculations. Construction of the 'convex hull' using DFT-calculated enthalpies of formation indicated that the phases expected at atmospheric pressure are Au, Au_5Na, Au_2Na, Au_2Na_3, $AuNa_2$ and Na. The DFT calculations also indicated that the Au_2Na structure could be stabilized by substitution of additional Na atoms on Au sites. The calculated enthalpies of formation for $Au_{2-y}Na$ lower and broaden the convex hull to the extent that formation of intermediate compounds such as Au_7Au_6 and AuNa would be unfavorable relative to $Au_{2-y}Na$ where $0 \leq y \leq 1$. We propose that the most straight-forward interpretation of the available data is that AuNa is not present at atmospheric pressure but that $Au_{2-y}Na$ and Au_2Na_3 are. We suggest that the currently available binary phase diagram is therefore incorrect. A revised binary phase diagram that is in agreement with the experimental and calculated data is provided.

Ferroelectric domain percolation in polycrystals

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Ferroelectric materials possess the ability to switch between polarization states on application of external fields. This switching is facilitated via movement of domains walls and is a critical factor in the performance metrics of these materials. Hence, the interaction of domain walls with microstructural features such as grain boundaries can influence their performance. Experimentally, domain continuity has only been observed over a few grains with no information of the domain percolation length in larger polycrystals. For domain continuity to be energetically feasible, conditions of ferroelectric polarization continuity and domain wall plane matching need to be satisfied at the grain boundary. In this work, we have studied the extent of continuity of domains within modelled polycrystals. It is shown that under tighter conditions of plane matching and uncompensated polarization charge, favorable grain boundary character can have considerable impact on the domain percolation. However, when the conditions of domain continuity are relaxed, due to higher charge and geometric tolerance, domain percolation throughout the polycrystal is a likely phenomenon. It is shown that percolation of domains through a polycrystalline ferroelectric could be tailored by microstructural control of the grain boundary types and defect chemistry control of the charge compensation mechanisms. The ability to manipulate the length-scale of correlated domain wall motion may lead to new opportunities in ferroelectric functional device design. Additionally, these results can be extended to study the effect of grain boundary character on other material phenomena that involve planar interactions at grain boundaries, including ferroelastic twin boundaries and slip plane continuity.

Micromagnets dramatically enhance effects of viscous hydrodynamic flow in two-dimensional electron fluid

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The hydrodynamic behaviour of electron fluids in a certain range of temperatures and densities is well established in graphene and in 2D semiconductor heterostructures. The hydrodynamic regime is intrinsically based on electron-electron interactions, and therefore it provides a unique opportunity to study electron correlations. Unfortunately, in simple longitudinal resistance measurements, the relative contribution of hydrodynamic effects to transport is rather small, especially at higher temperatures. Viscous hydrodynamic effects are masked by impurities, interaction with phonons, uncontrolled boundaries and ballistic effects. This essentially limits the accuracy of measurements of electron viscosity.

Fundamentally, what causes viscous friction in the electron fluid is the property of the flow called vorticity. In classical fluids, vorticity is generated by non-uniformities in the velocity profile caused by boundaries and regions of high vorticity are confined to boundary layers. In this work we propose to use micromagnets to exploit the charged nature of the electron fluid to drive non-uniform flow in the bulk. With the vorticity no longer confined to the boundary regions, the vorticity, and therefore viscous dissipation, is increased by orders of magnitude. Experimental realization of this proposal will bring electron hydrodynamics to a qualitatively new precision level, as well as opening a new way to characterize and externally control the electron fluid.

Universality Classes Across the Paramagnetic Transition in the Skyrmion Material $Cu_2OSe_{1-x}Te_xO_3$

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Since the discovery of Skyrmions in the chiral multiferroic material Cu_2OSeO_3, the stability and formation of Skyrmion spin textures has been presumed to be due to a competition between the Dzyaloshinskii-Moriya interaction and exchange interaction, which is thought to be Heisenberg-type above and below the paramagnetic transition[1]. However, recent analysis shows that highly anisotropic systems can exhibit different universality classes on either side of a phase transition[2], leading to claims that the exchange interaction transitions from the Heisenberg to Ising universality classes as the temperature drops below T_c[3].

We present preliminary scaling results in agreement with this Heisenberg to Ising transition for an undoped Cu_2OSeO_3 sample. However, we also present an analysis of a $Cu_2OSe_{1-x}Te_xO_3$ for $x \sim 0.2$. The inclusion of the Te ions expanded the unit cell by 0.1% and decreased the magnetic phase transition by ~3K. We find that there is no agreement with any known universality class above the transition and present several possible causes for this result. Particular attention is paid to the role of the demagnetising field and its correction, as well as outlines of future experiments to investigate further the relationship between doping, magnetic anisotropy, and universality classes in this material.

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Aspects of the Physics of Palladium Di-Telluride

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For many years Solid State (and now Condensed Matter) Physicists have been fascinated by crystalline materials displaying crystal structures of "less than three dimensions". A classic group of such materials are the transition-metal di-chalcogenides (TMDCs) which exhibit a range of most interesting properties. The appearance of superconductivity amongst this group was excellently review by Wilson and Yoffe [1]. These compounds, with the general formula MX_2, consist of a group-IV to -VIII metal, *M*, and a chalcogen atom, *X* (S, Se, or Te) and they crystalize in various polytypes composed of *X*-*M*-*X* sandwiches. In general, for the superconducting members, the *M*-*X* coordination is trigonal prismatic. $PdTe_2$ is the notable exception to this general rule since for it the *M*-*X* coordination is octahedral.

As can happen, by "good fortune", a single crystal sufficiently large for a neutron triple-axis experiment, was prepared and as a result the phonon dispersion curves along the [ζ00], [ζζ0] and [00ζ] symmetry directions were successfully measured, enabling the data to be fitted quite well with a lattice-dynamical model consisting of axially symmetric, Born-von Kármán interactions together with shell-model contributions, introduced specifically to model dips in the low-energy optic branches [2].

But recently, there has been much interest in $PdTe_2$ as a possible candidate for exhibiting topological superconductivity [3,4,5].

In this poster presentation, aspects of the lattice dynamics will be discussed, together with heat capacity data which would indicate that $PdTe_2$ is a "conventional", BCS superconductor.

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Evolution of local short-range order of liquid metals under static magnetic field

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Gallium is a fascinating metallic element that melts at around room temperature (T_m = 302.9 K) and keeps the liquid state till supercooled to 270 K, which endows it with complex solid and liquid characteristics. Its extraordinary physicochemical properties have resulted in gallium and liquid metal alloys based on it being applied in many fields, like flexible liquid robotics [1] or biomaterials [2]. Our research aims to reveal the effects of static magnetic fields (SMF) on gallium-based liquid metals on atomic scales. The study will provide the principal support for the future liquid metals' applications under magnetic field environments. We performed high-energy X-ray diffraction experiments (Shanghai Synchrotron Radiation Facility) and, utilizing a portable electromagnet, we studied the local atomic order of the liquid metals under SMF (0.2 T). Concurrently, we have developed a molecular dynamic simulation-assisted reverse Monte Carlo program (MD@RMC) to reconstruct the atomic configuration from the X-ray structure factor results. Furthermore, Voronoi polyhedral and bond-orientational order parameters were applied to analyze the local short-range order (LSRO). The results of the experiments and simulations indicate that application of SMF has a measurable influence on LSRO distribution. Specifically, SMF disorders the system and drives it form localized atom clusters of lower coordination number.

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Theoretical modelling on new level crossings and electron-hole asymmetry in Landau octet of bilayer graphene

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The highly tunable band structure and eightfold degeneracy of the zero-energy Landau level (zLL) of bilayer graphene (BLG) make it an ideal platform for engineering new quantum Hall states, denoted by the orbital, valley, and spin quantum numbers. However, determining the orbital, valley, and spin order of quantum Hall states at different filling factors and electric fields is still an unresolved question. In the experiments, we observe new zero-energy Landau level crossings at filling factor -2, 1 and 3 in high electric fields at millikelvin temperatures. These observations enable us to constrain the parameters for constructing a simplified effective single-particle theoretical model, which can be used to fully determine the quantum Hall states. The model predicts the importance of coulomb interactions in this system via exchange-enhanced Zeeman g-factor.

Anderson's Theorem and Superconducting Fitness in Multiband Superconductors

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There has recently been much interest in a generalised Anderson's theorem for odd-parity superconducting states in strongly spin-orbit-coupled materials. In this talk we consider a minimal model of such a system based on a bilayer with Rashba spin-orbit coupling. We investigate the spectrum of the bound states around an isolated impurity using numerical self-consistent mean-field theory and an analytic non-self-consistent T-matrix theory. We find excellent agreement between the two methods, which reveals that the main features of the bound state spectrum are fixed by the "fitness" of the pairing state with respect to the impurity potential and the normal-state electronic structure. We generalise our theory to a three-dimensional nodal superconductor and show that the bound state spectrum largely survives as virtual bound states. Our analysis reveals the central role of the superconducting fitness in underpinning the generalised Anderson's theorem.

*N.A.H. and Y.Z. contributed equally to this work.

Low temperature magnetism in $TmNiAl_4$

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This paper will detail a study of the rare earth intermetallic $TmNiAl_4$ via ^{169}Tm Mössbauer spectroscopy plus specific heat and magnetometry. Analysis of the Mössbauer spectra reveals a Tm^{3+} magnetic hyperfine field (672(10) T) close to the free ion value of 663 T [1], suggesting a ground state consistent with fully stretched J = 6. The bulk measurements show a magnetic transition at 4.9 K. This transition is assigned as the Néel temperature on the basis of the magnetometry and similar antiferromagnetic behaviour observed in numerous other $RNiAl_4$ compounds such as $TbNiAl_4$ [2,3]. The persistence of magnetically-split Mössbauer spectra to well above this $T_N = 4.9$ K is consistent with a slow Orbach type paramagnetic relaxation that proceeds via the third excited crystal field level. The temperature dependence of the experimentally determined relaxation times positions this excited state at □ ≈ 360 (20) K above the ground state.

An understanding of remarkable nature of the metamagnetic behaviour of $TbNiAl_4$ with two distinct ordered phases was made possible by study of single crystals. Other $RNiAl_4$ compounds such as with R = Pr, Gd and Dy are also known to show the similar behaviour of two distinct metamagnetic transitions. However, a possible second transition in $TmNiAl_4$ is still an open question. New evidence in the form of heat capacity and magnetometry on polycrystalline $TmNiAl_4$ down to 0.5 K still leaves the door ajar.

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Study of the Crystal structures and magnetic properties of Sr_2RENbO_6 double perovskites.

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Crystal structures and magnetic properties of double perovskite (DP) Sr_2RENbO_6 (RE = Gd, Tb, Dy, Ho, Er and Tm) are investigated. The samples were prepared via ceramic solid-state reaction and crystal structures were confirmed by X-ray powder diffraction (XRD). The XRD results having been refined to confirm the crystal structure by Rietveld refinement (using Fullprof [1]). All samples of Sr_2RENbO_6 double perovskite are single phase with monoclinic symmetry, space group $P2_1/n$ space group (No.14) [2].

DC magnetisation as a function of temperature and magnetic field were measured using a Physical Property Measurement System (PPMS) from 1.8 to 295 K for all samples. The Sr_2RENbO_6 DP compounds display Curie–Weiss paramagnetic behaviour and show effective paramagnetic magnetic moments which are in good agreement with the RE^{+3} free ion values [3]. Of particular note from the DC magnetisation results of is the observation of field induced magnetic order across the series, noted via a dip in the differential of the data that is seen to shift to higher temperature with increasing magnetic field (in the range 0.2 to 5 T).

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Koopmans' integral and perturbative optoelectronic properties of the perovskite Cs_2TiBr_6 for sustainable energy conversion

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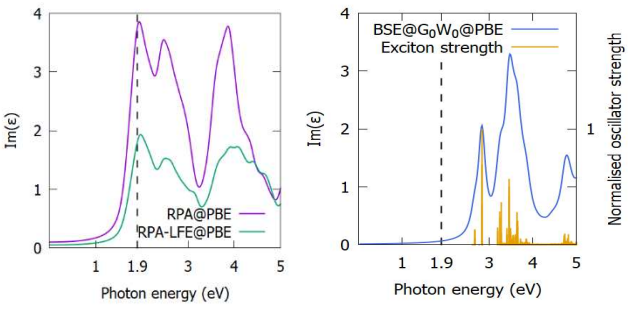
Transformational change is required to address the impacts of human-induced climate change. During the previous decade there has been a rapid increase in the power conversion efficiency (PCE) of thin-film solar cells based on a hybrid organic-inorganic halide perovskite absorbing layer to ~25%. However, lead toxicity and stability remain barriers to commercialisation. The vacancy-ordered double perovskite (VODP) structure of all-inorganic compounds offer advantages of increased stability and an enlarged compositional space to facilitate element substitution. For example, Cs_2TiBr_6 thin film provides a stable, non-toxic absorbing layer composed of abundant elements with a first attempt PCE of 3.3% [1].

In contrast to conventional semiconductors, there is evidence to suggest the polaronic trapping in the halide perovskites facilitates the spatial separation of excited charge carriers, resulting in decreased recombination rates combined with moderate carrier mobilities. In addition, excitons with short lifetimes can facilitate efficient absorption of solar radiation.

The aim of this work is to further understand the optoelectronic and quasi-particle properties of stable lead-free VODPs for sustainable energy conversion. Optoelectronic properties of Cs_2TiBr_6 are determined here using a range of computational techniques, including a state-of-the-art Koopmans' Integral functional (KI) for accurate spectral properties [2]. KI restores piecewise-linearity of the total energy with electron number to Kohn-Sham DFT. The G_0W_0 method of Many-Body Perturbation Theory (MBPT) provides quasi-particle band structures with exciton energies from the Bethe-Salpeter Equation (BSE) [3]. Experimental band gaps for bulk Cs_2TiBr_6 have been reported as 1.78 eV [4], 1.9 eV (indirect) and 2.0 eV (direct) [5].



The KI functional shows an PBE fundamental band gap E_g = 4.02 eV in accord with a fully relativistic G_0W_0 gap of 3.66 eV. The imaginary part of the dielectric function, calculated with the random phase approximation (RPA) shows strong local field effects (LFE), and an optical absorption onset in agreement with experimental band gaps. Further, the BSE@G_0W_0 computation shows optical absorption from low energy Frenkel excitons, reducing the band gap from 3.66 eV to 2.8 eV. Preliminary results show polarons as charge carriers that are self-trapped and screened within local distortion of the ionic lattice. Thus, additional polaron binding energy or phonon zero-point renormalisaton can possibly reconcile the BSE@G_0W_0 band gap with experiments.

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Towards an all-diamond superconducting platform

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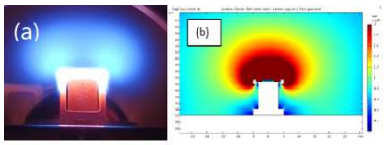
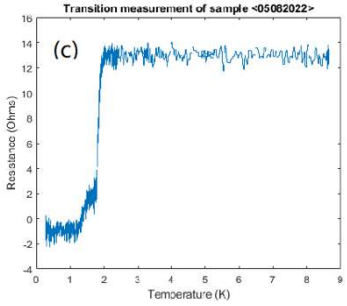
The discovery of superconductivity in boron doped diamond opens a pathway to a monolithic device providing the challenges of growth and fabrication can be overcome. Superconducting quantum devices have already been developed with many applications. This includes, for example, SQUIDs for sensing magnetic fields for mining industry from the CSIRO and quantum chips have been developed by IBM and Google. Coupling a qubit to a resonator circuit may offer novel qubit programming and read-out schemes. Resonator circuits are traditionally fabricated from aluminum or niobium on low dielectric loss substrates such as silicon or sapphire. Such fabrication processes are well developed and have already been utilized in complicated, large-scale device geometries. However, the performance of such superconducting devices is largely limited by charge noise and losses from two-level states arising at the interfaces between the substrate, superconducting metallization, and vacuum, as well as the intrinsic dielectric loss of the substrate.





These problems can potentially be avoided in a monolithic diamond device. Diamond exhibits electrical p-type conductivity when doped with boron, and superconductivity at liquid helium temperature when the boron concentration exceeds the metal-insulator transition concentration of $3 \times 10^{20}\ cm^{-3}$ [1]. Its critical temperature can exceed $10\ K$ for (111) oriented substrates, $4\ K$ for (100) oriented substrates, and it is a type-II superconductor with upper critical field above $10\ T$ [2]. Moreover, un-doped diamond is strongly tolerant to oxidation, highly insulating and exhibits a low dielectric loss tangent. Superconducting boron doped diamond can be epitaxially grown on top of insulating diamond substrates by employing chemical vapor deposition (CVD). These films could result in an all-diamond homostructure that eliminates material interfaces, with the potential to reduce the dielectric losses and electric field noise that limit existing implementations.

We have investigated the optimum CVD growth parameters by placing substrates in novel 3D-printed titanium cages that enhance the boron content and uniformity of the films during growth. Our optimization process has been guided by CMOSOL simulations of the boron concentration in the gas phase as a function of the cage geometry. This paper reviews our extensive studies in growing CVD boron doped diamond films on readily available (100) substrates with a superconducting critical temperature of $1.8\ K$ (see figure).

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Designing Better Electrodes with Electrochemical Microscopy

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All solid surfaces—from the simplest monocrystals to the most complex composite nanomaterials—possess some degree of heterogeneity but determining how surface structure affects electrode functional properties (e.g., catalytic activity, selectivity, stability etc.) can often be challenging using traditional "bulk" electrochemical techniques. Scanning electrochemical probe microscopy (SEPM) is a nanopipette-based scanning probe microscopy (SPM) technique to measure and visualise electrochemical (electrocatalytic) activity with high spatiotemporal resolution. This presentation will spotlight the use of SEPM for probing the electrocatalytic activity of nanomaterials on a commensurate scale to surface structural heterogeneities (i.e., nm–μm scale). It will be demonstrated that this approach is widely applicable to: well-defined monocrystals (e.g., transition metal dichalcogenides: MoS_2; Fig. 1a) [1]; structurally heterogeneous polycrystals (e.g., polycrystalline Au and Cu, etc.; Fig. 1b) and [2,3]; composite nanoparticle-on-support "ensemble" electrodes (e.g., nanoparticles/platelets supported on carbon; Fig. 1c) [4]. In particular, it will be emphasised how nanoscale-resolved information from SEPM is readily related to electrocatalyst structure and properties, collected at a commensurate scale with complementary, co-located microscopy/spectroscopy techniques (e.g., SEM, TEM, EBSD, AFM etc.), to allow structure−activity relationships to be assigned directly and unambiguously.

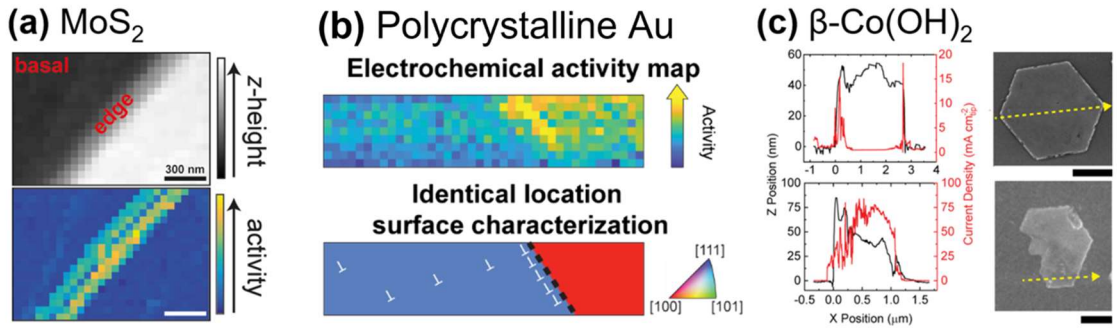

Fig. 1. Structure−activity correlations for (a) MoS_2, (b) polycrystalline Au and (c) β-$Co(OH)_2$ nanoplates (supported on glassy carbon).

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Optical and Electron Energy Loss Spectroscopy (EELS) with Density Functional Theory: The Independent Particle Approximation and Beyond

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The ability of density functional theory (DFT) to provide insight into many materials properties is one of the great successes of condensed matter physics. However, excited state properties, such as optical responses, remain an ongoing challenge from both a computational and theoretical standpoint. In the simplest approximation, the independent particle approximation (IPA), the electron and hole generated are assumed to not influence the other electron states and do not interact with one another. That is, quasiparticle and excitonic effects are ignored. This approach works for some systems but is a poor approximation for many others. Sometimes the inclusion of local field effects (LFE) are important and sometimes computationally expensive approaches can be avoided by using alternative exchange-correlation potentials instead.

EELS is another spectroscopic technique for measuring optical response functions but with the additional benefit of being able to obtain information at the nanometre scale. However, the large energy range typical for EELS data puts unique demands on the computational processing required and careful selection of the appropriate level of calculation is necessary.

This presentation will demonstrate the applicability of various levels of computation to modelling optical properties and electron energy loss spectroscopy (EELS) for a range of different materials.

Nonlinear Quantum Electrodynamics in Dirac materials

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Classical electromagnetism is linear. However, fields can polarize the vacuum Dirac sea, causing quantum nonlinear electromagnetic phenomena [1], e.g., scattering and splitting of photons, that occur only in very strong fields found in neutron stars or heavy ion colliders. We show that strong nonlinearity arises in Dirac materials at much lower fields ∼1 T, allowing us to explore the nonperturbative, extremely high field limit of quantum electrodynamics in solids. We explain recent experiments in a unified framework and predict a new class of nonlinear magnetoelectric effects, including a magnetic enhancement of dielectric constant of insulators and a strong electric modulation of magnetization. We propose experiments and discuss the applications in novel materials. [2]

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Observation of artificial bandstructure in a patterned semiconductor two-dimension electron gas

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The electronic properties of materials are determined by their crystal structure and the type of atoms. Engineered metamaterials, which are created by imposing external spatially-periodic potential, a superlattice, have offered a tool to alter materials properties beyond those found in nature. A spectacular example is Moire superlattices, where different layers of two-dimensional (2D) materials are stacked and twisted to create a superlattice modulation potential, are currently attracting significant attention as they provide an ideal platform for both studying fundamental physics as well as promising future applications. Imposing spatially periodic electric field via nanoscale patterning has also been proven to be a powerful technique to create a superlattice. It offers an excellent control of the lattice parameters and can be easily integrated into many existing device architectures, including conventional semiconductor FETs, which have an advantage of well-established fabrication technology and superb device quality.

In this study, we exploit the technique of gate patterning to fabricate an accumulation mode FET based on a high quality shallow GaAs heterostructure. By measuring quantum oscillations in the magnetoresistance, we identify multiple artificial Fermi surfaces induced by the gate patterned superlattice. Furthermore by changing the gate bias we are able to increase the strength of the modulation potential and observe sign changes of the Hall slope, which is direct evidence of the formation of artificial energy bands. Our results demonstrate that gate-patterned superlattices combined with shallow semiconductor heterostructures can serve a powerful tool to engineer and study artificial energy bands.

Microscopic theory of the effect of backscattering on the electronic and optical response of graphene

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The optical conductivity of graphene results from an interplay between intraband and interband transitions [1, 2]. The former process usually dominates in the THz frequency range and can be described by the Drude model. However, in some cases, the THz response of graphene deviates from the Drude formula [3]. This effect is usually associated with backscattering and can be phenomenologically described by the Drude-Smith model [4]. In this work, we propose a more rigorous and accurate theory based on the density matrix theory [5] and semiconductor Bloch equations [6] to describe the interplay between backscattering, electron-phonon scattering, and the optical response of graphene.

Unlike the Drude-Smith model, the proposed microscopic theory gives accurate predictions for dependencies of the optical conductivity spectrum on temperature and doping level. Our findings show, that, at room temperature in the THz frequency range, the backscattering can lead to the coherent coupling between the photon-assisted non-direct transitions and direct interband transitions This effect manifests itself as a deviation of the conductivity spectrum from the Drude model and as an enhancement of the interband absorption compared to the intraband one.

The results of modeling have been verified experimentally by measuring the complex dynamic conductivity using the time-domain THz spectroscopy applied for CVD-grown graphene (deposited on a SiO_2/p-doped Si heterostructure). The SiO2 substrate represents a source of the elastic scattering centers in graphene and causes backscattering for electrons accelerated by the THz electromagnetic field. The conductivity spectra have been measured at room temperature in the frequency range 0-8 THz as a function of the gate voltage controlling the doping level.

[1] H.A. Hafez, et al., *Adv. Optical Mater.*, **8**, 1900771 (2020)
[2] P. Gallagher et al., *Science* **364**, 158 (2019)
[3] J.D. Buron et al., *Nano Lett.* **14**, 11, 6348 (2014)
[4] H.J. Joyce et al, *Semicond. Sci. Technol.* **31,** 103003 (2016)
[5] H. Haug and S.W. Koch, *Quantum Theory of the Optical and Electronic Properties of Semiconductors*, (World Scientific, 2004) p.453
[6] H. Kitamura, Eur. J. Phys. **36** 065010 (2015)

Patterned bilayer graphene as a tunable, strongly correlated system

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Recent observations of superconductivity in Moire graphene [1] have lead to an intense interest in that system, with subsequent studies revealing a more complex phase diagram including correlated insulators and ferromagnetic phases. Here we propose an alternate system, electrostatically patterned bilayer graphene (PBG), in which a supermodulation is induced via metallic gates rather than the moire effect. We show that, by varying either the band gap or the modulation strength, bilayer graphene can be tuned into the strongly correlated regime. Further calculations show that this is not possible in monolayer graphene. We present a general technique for addressing Coulomb screening of the periodic potential and demonstrate that this system is experimentally feasible. While the work presented here is theoretical, it is also of experimental interest.

[1] Cao, Yuan, Valla Fatemi, Shiang Fang, Kenji Watanabe, Takashi Taniguchi, Efthimios Kaxiras, and Pablo Jarillo-Herrero. "Unconventional Superconductivity in Magic-Angle Graphene Superlattices." *Nature* 556, no. 7699 (April 2018): 43–50. https://doi.org/10.1038/nature26160.

Theory of emergent inductance: effect of nonlinearity

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Emergent electromagnetism in magnets originates from a nontrivial Berry phase due to strong coupling between spins of conduction electrons and non-collinear magnetic moments. This offers possibilities to develop new functionalities associated with quantum transport and optical responses. The emergent inductance [1, 2, 3] in spiral magnets is one of the most intriguing phenomena resulting from the emergent electric field, which has been recently experimentally confirmed [4, 5]. The experimentally observed inductance is around ∼100nH, which is comparable to the best commercial values, while the size of the sample is $\sim 10^{-5}$ smaller.

We introduce a theory of the emergent inductance in spiral magnets, which explains its magnitude, sign, frequency dependence, and nonlinearity. We analytically study the effect of nonlinearity in emergent inductance based on the dynamics of collective excitations in spin spirals. Furthermore, our micromagnetic simulations confirm the nonlinearity and sign change of the inductance, which agree well with experimental observations. Our theory provides a fundamental understanding of the phenomenon and opens a way to design emergent nanoscale inductors.

[1] N. Nagaosa, *Jpn. J. Appl. Phys.* **58**, 120909 (2019).
[2] J. Ieda, and Y. Yamane, *Phys. Rev. B* **103**, L100402 (2021).
[3] D. Kurebayashi and N. Nagaosa, *Commun. Phys*. **4**, 260 (2021).
[4] T. Yokouchi, et al. *Nature* **586**, 232-236 (2020).
[5] A. Kitaori, et al. *Proc*. *Natl. Acad. Sci. U.S.A.* **118**, e2105422118 (2021).

X-ray absorption spectroscopy at the Australian Synchrotron for materials characterisation

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In this presentation, X-ray absorption spectroscopy (XAS) in the context of the Australian Synchrotron will be presented, along with several examples of materials characterisation using the different techniques available to scientists that use the facilities.

XAS is characterisation technique that is largely used to probe the chemical (oxidation) state of elements of interest. XAS does this by analyzing the how the interaction of x-ray with the element of interest changes with changes to the incident photon energy. The most basic of techniques is transmission XAS, where the incident photon energy is scanned from below the energy needed to excite the target elements core electrons to above the energy, resulting in spectra showing the change in absorption of the sample with photon energy.

While XAS has historically been a synchrotron technique, there are now several companies that produce lab-based XAS instruments. With the commissioning of the new medium (or tender) energy x-ray absorption spectroscopy beamlines (MEX/TEX), the Australian Synchrotron can core shell energies (k-edge) of most elements of interest to the scientific community (Be to Sb).

Within XAS, there are several different types of analysis that can be conducted. The Soft X-Ray (SXR) beamline covers the energy range of 0.1 to 2.5 keV (k-edges of Be to S). Soft x-ray measurements are conducted at ultra-high vacuum and are highly surface sensitive techniques. This surface sensitivity can also be used to investigate the chemical states of metals above Al using the higher shells of L and/or M. In addition, the SXR beamline has access to an Angle-resolved photoemission spectrometer, which will be presented by Dr. Anton Tadich at this conference. The MEX2 beamline also conduct some measurements at vacuum and be surface sensitive in the energy range of 1.8 to 3.2 keV and has been tailored to investigate the core electron chemical states of silicon, phosphorus and sulphur.

MEX1 and the XAS beamlines are tender to hard energy x-ray beamlines and are bulk spectroscopy techniques. While not being as surface sensitive, the higher penetrating power of x-rays enable routine in-situ studies of materials, including batteries, solar cells, and catalyst materials among others. In addition, extended x-ray absorption fine structure (EXAFS) can be conducted at MEX1 and XAS, which can measure the interatomic distances and co-ordination numbers in materials regardless of long-range order or crystallinity.

Stoichiometric hydration of interstitial sites in a close-packed ionic lattice

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The hexagonal perovskite-type oxide 6H-$Ba_4Ta_2O_9$ undergoes an unconventional symmetry lowering lattice distortion when cooled below 1100 K in the presence of atmospheric water. This temperature corresponds to the onset of hydration, which reaches a stoichiometric value 6H-$Ba_4Ta_2O_9.½H_2O$ by ~500 K. We have used a combination of diffraction, *ab initio* calculations and spectroscopy to show that both processes are due to the incorporation of intact water molecules into the close-packed ionic lattice. The presence of very large Ba^{2+} cations in octahedral interstitial sites (perovskite *B* sites) forces adjacent vacant octahedral interstitial sites to also expand, making room for occupation by water molecules, while also destabilizing the structure in a way that cannot be adequately addressed by conventional symmetry lowering pathways on cooling. This gives rise to a synergistic hydration-distortion mechanism, which, to the best of our knowledge, is unique among close-packed ionic compounds.

Nanoscale design to make materials surpass themselves

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In traditional condensed matter physics, we have learnt many about how the crystal structure will determine the property and function of materials. On the other hand, our research suggests that the local structure of materials may be different from the average structure defined by X-ray crystallography. This gives us a hint to chemically and structurally engineer the materials at various length scales to create new properties and functions that have never been expected to be seen in such materials. In this talk I will show how to overcome the limitation of traditional dielectric and ferroelectric materials, and achieve new capabilities far beyond occurrence, which also theoretically enrich condensed matter physics.

Characterising Magnetic Nanoparticles: the Infamous Blocking Temperature and Interaction Temperature

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Magnetic nanoparticles are used to heat and kill cancerous tumors, to image biological tissues, to shield electromagnetic radiation, and are even used in self-healing paints. For state-of-the-art technologies, magnetic nanoparticle materials must be well-characterised and understood before use. This is particularly true for emerging biomedical applications so that patients are not harmed but indeed helped by these materials. There are two key parameters for characterizing magnetic nanoparticles: the blocking temperature and the interaction temperature.

The **blocking temperature** is the mean temperature at which the magnetization of a nanoparticle system transitions from being stuck in a local energy minimum (low temperatures, "blocked" state) to being free to visit all angles (high temperatures, "superparamagnetic" state). In other words, it is a measure of the height of magnetic energy barriers. Recently, we showed theoretically that the blocking temperature can be determined from magnetization versus temperature measurements and that it is lower than what many researchers currently claim it to be. [1] The word needs to get out: the blocking temperature is easy to calculate… but one should use the correct model to do so! [2]

The **interaction temperature** is a measure of how strong dipolar interactions are between magnetic nanoparticles. Just like fridge magnets, tiny nano-magnets attract and repel one another from a distance. A single magnetic nanoparticle feels a net dipolar magnetic field produced by its many neighbours. However, this net field is difficult to calculate because dipolar fields are long ranged and point in all different directions. In this talk, how the interaction temperature is inferred from magnetization versus temperature measurements will be explained. Then, results of numerical calculations will be presented which show that the "interaction temperature" may also depend strongly on factors beside the dipolar interaction strength! [3] In that case, we should tread cautiously and re-examine existing data on magnetic nanoparticles.

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[2] I.J. Bruvera, P. Mendoza Zélis, M. Pilar Calatayud, G.F. Goya and R.H. Sánchez, *J. Appl. Phys.* **118**, 184304 (2015).
[3] R.E. Camley, R. Macêdo, A.R. Chalifour and K.L. Livesey, *in preparation.*

Magnetism in epitaxial thin films of the high entropy oxide $La(Cr_{0.2}Mn_{0.2}Fe_{0.2}Co_{0.2}Ni_{0.2})O_3$

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Information technologies account for approximately 8% of global energy use and are projected to account for up to 14% of global greenhouse gas emissions by 2040 [1]. Operating on electron spin instead of charge, spintronic devices offer fast, non-volatile, and energy efficient computing and memory [2]. The importance of these technologies is growing not only due to the environmental and economic impacts of high energy usage, but also because current technologies are reaching their physical limits (e.g. due to Boltzmann's Tyranny), limiting computational power [3]. $La(Cr_{0.2}Mn_{0.2}Fe_{0.2}Co_{0.2}Ni_{0.2})O_3$ is a high entropy perovskite oxide which has attracted interest due to the ability to switch between antiferromagnetic and ferromagnetic ground states by varying its Mn concentration [4]. By targeting the boundary between these two states, it may be possible to use other external stimuli to switch between antiferromagnetism and ferromagnetism, allowing for new spintronic functionality. It has been proposed that this switching behaviour is due to competition between the fifteen different exchange interactions in this material[4]. By growing thin films of $La(Cr_{0.2}Mn_{0.2}Fe_{0.2}Co_{0.2}Ni_{0.2})O_3$, we aim to investigate how the interplay between competing interactions in these epitaxial thin films can be used to engineer magnetic properties through finely controlling stoichiometry, thickness, strain, and thin film heterostructures. We have synthesized this material with varying concentration of Mn and suggest that this leads to a mixed ferro- and antiferromagnetic phase based on preliminary bulk powder magnetometry results. We also demonstrate that this high-quality thin films of this material grow epitaxially on $SrTiO_3$, $LaAlO_3$, and $NdGaO_3$ substrates based on atomic force microscopy and X-ray diffraction measurements.

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2. Manipatruni, S., et al., *Scalable energy-efficient magnetoelectric spin–orbit logic.* Nature, 2019. **565**(7737): p. 35-42.

3. IEEE, *Beyond CMOS*, in *International Roadmap for Devices and Systems (IRDS™) 2020 Edition*. 2020, IEEE.

4. Mazza, A.R., et al., *Designing Magnetism in High Entropy Oxides.* Advanced Science, 2022. **9**(10): p. 2200391.

Analytic Theory for Magnetic Skyrmions

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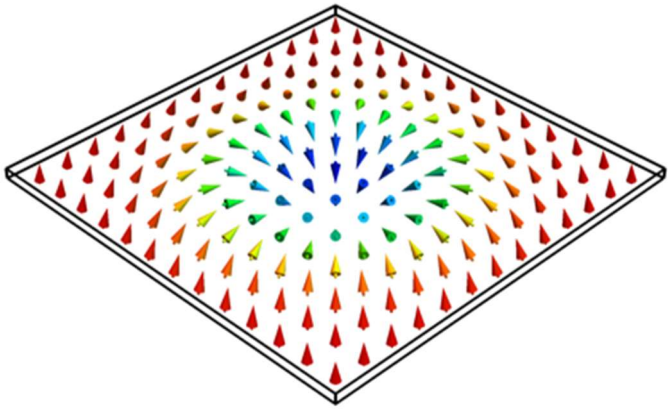
Magnetic skyrmions are tiny swirls in the direction of the local magnetization. This is shown in the illustration to the right, where the coloured arrows represent the local magnetization direction within a magnetic thin film containing a skyrmion. Skyrmions are as small as a few nanometres wide and can be moved around inside a magnetic film or wire using very low energies, making them of interest for data storage and computing applications.



In this work, we have developed a semi-analytic theory to predict the size of a skyrmion in a given magnetic thin film and with a given applied magnetic field. This is done by assuming a linear approximation for the magnetisation variation as a function of the radial distance from the centre of the skyrmion, and by then minimising the total energy. It also makes use of a Green's function approach to calculate the demagnetising energy contribution.

Our results are compared to those from micromagnetic simulations to ensure their accuracy. They are also compared to those from other approximate analytic calculations. [1,2] The key is that our analytic prediction saves a great deal of time compared to running lengthy simulations, plus allows one to see the dependence of the skyrmion size on different magnetic parameters. Moreover, it is more accurate than one commonly-used calculation [2] and is simpler to use than another. [1]

[1] F. Büttner, I. Lemesh and G.S. Beach, *Sci. Rep.* **8**, 4464 (2018).
[2] X.S. Wang, H.Y. Yuan and X.R. Wang, *Commun. Phys.* **1**, 1 (2018).

Neutron Polarisation at the Australian Centre for Neutron Scattering

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The ability to determine the influence of neutron spin on their interaction with matter can in many cases reveal unique information in studies of scattering processes. Six of the neutron scattering instruments at the Australian Centre for Neutron Scattering (ACNS) offer the ability to perform polarisation analysis experiments [1], where neutron spin both before and after the sample can be manipulated and filtered. This allows measurements which study magnetic structures or separate coherent and incoherent scattering to be performed under a wide range of conditions. An overview of these capabilities will be given, along with a description of some upcoming new capabilities spanning a variety of setups.

[1] W. T. Lee and T. D'Adam, *Neutron News* **27**, 2 (2016).

Not Nitrogen-Vacancy Centre in diamond again

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The nitrogen adjacent to a vacancy (NV) in diamond behaves like a 'molecule' embedded in diamond. The molecule can exist in two charge states, neutral NV^0 and negative NV^- with the majority of interest in the latter because of properties that lead to may applications – detection of magnetic fields, electric fields, strain or temperature. The properties and in particular the interchange between NV^0 <-> NV^- depend on the local environment and this is the focus here.

There is nearly almost always some nitrogen incorporated in diamond. When there is very little nitrogen (parts per billion) it is hard but possible to obtain the negative charge state. Once formed with no additional nitrogen close the NV^- is reasonably stable. This is the situation for many applications and termed 'single NV'. It can be optically transformed between NV^- and NV^0 but the transitions involve electrons or holes from valence or conduction band.

The situation is different when there is a density of nitrogen in the crystal. The difference being there is readily available donor electrons from the nitrogen in the local environment. In this situation electrons can move between the NV and the adjacent nitrogen without involve valence or conduction electrons. The transitions are spontaneous via tunnelling to obtain lower energy. Photons can be involved but this is to access a different state. Once in that state the charge transfer itself is spontaneous.

There is a difference for 'single NV' the NV^0 <-> NV^- charge transfer is optically driven whereas with nitrogen present the transfer is spontaneous. 'Games are played' with these charge transfer processes for many applications and can be complicated as light can switch both ways. There are an enormous number of publications involving NV and the change of charge state of NV can be important. Where change of charge state is treated the majority only consider the 'single' processes and do not recognize that if the local environment involves nitrogen extra processes can occur and totally alter the situation. Can be confusing for reader!

Neutron Laue Diffraction – A Spotted History, a Scintillating Future

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In 1912, Max von Laue first demonstrated atomic diffraction produced by passing a beam of polychromatic X-rays through a single crystal. Laue diffraction, as this phenomenon was later called, was also demonstrated with neutrons, shortly after the pioneering monochromatic experiments by Schull and co-workers at Oak Ridge in the 1940s. The Laue technique then languished for many decades, due to the perception that harmonic overlap and complicated wavelength-dependent corrections gave data of lesser quality than monochromatic diffraction.

The extreme demands of protein crystallography for higher data collection rates, for both X-rays and neutrons, coupled with high-resolution, large area detectors, and powerful image-analysis techniques, allowed Laue diffraction on a continuous source of radiation to return to the forefront of crystallography in terms of increasing unit-cell size, decreasing sample volume, and higher-throughput experiments. Modern reactor-based neutron Laue diffractometers with large image-plate detectors permit extensive continuous sampling of reciprocal space with high resolution in the two-dimensional projection and a wide dynamic range with negligible bleeding of intense diffraction spots, qualities that are highly suited to detection of incommensurate structures, high-pressure crystallography, and diffuse scattering.

Although time-of-flight neutron diffraction on a white beam was first demonstrated at the Dubna pulsed reactor in 1964, it was not until a position-sensitive (scintillation) detector became available that the full utility of the technique for single crystals could be realised in a landmark experiment at IPNS in 1984. Using a scintillator gave negligible parallax, which allowed the detector to be moved close to the sample to increase significantly the solid angle of detection to make the data-collection efficiency comparable to that on a monochromatic diffractometer with a point detector at a reactor source. Such detector developments will continue to play a key role in broadening the application of neutron Laue diffraction.

A survey of pioneering studies of neutron Laue diffraction at reactors and spallation sources guides us to what we may achieve with upcoming instrumental and data-analysis advances.

Strongly-correlated superconductivity with spin-orbit coupling

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Motivated by the recent discovery of a field-mediated parity switch within the superconducting state of $CeRh_2As_2$ [1], we investigate the superconducting phase diagram of a strongly-coupled Rashba mono- and bilayer. Our model extends the usual two-dimensional Hubbard model by including Rashba spin-orbit coupling due to broken inversion symmetry, and interlayer hopping in the case of the bilayer. The strong correlations due to the on-site repulsion are accounted for within the auxiliary boson mean-field theory.

We find that the usual *d*-wave solution is replaced by an extended *s*-wave state at sufficiently large interlayer hopping or spin-orbit coupling strength. Including an applied magnetic field we observe a transition to an exotic "staggered singlet" odd-parity state, recalling the phase diagram of $CeRh_2As_2$.

[1] S. Khim, J. Landaeta, J. Banda, N. Bannor, M. Brando, P. Brydon, D. Hafner, R. Küchler, R. Cardoso-Gil, U. Stockert, et al., *Science* **373**, 1012 (2021).

Electric-field-control of THz conductivity in graphene: from Drude to non-Drude regime

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Due to its outstanding electrical, optical and mechanical properties, as well as the accessibility of synthetic large-area films, graphene offers potential for a wide range of technologies, from electronics to optoelectronics and sensing. In particular, the electronic properties of graphene can be tuned via electrostatic gating, by applying an external electric field which alters its charge carrier density and electrical conductivity. Terahertz time-domain spectroscopy (THz-TDS) allows for measuring the complex dynamic electrical conductivity $\tilde{\sigma}(\omega)$ resulting from charge carrier dynamics in a variety of materials. While $\tilde{\sigma}(\omega)$ for metallic graphene (i.e., doped, with the Fermi level E_f far from the Dirac point) has been well characterized and explained within the few-THz spectral range by Drude-type models, these models fail to quantitatively describe the full complex $\tilde{\sigma}(\omega)$ (i.e., real and imaginary parts) of charge neutral graphene (i.e., with E_f at the Dirac point) within a broad ~10 THz spectral window.

In this work, we measured the complex dynamic conductivity $\tilde{\sigma}(\omega)$ of CVD-grown graphene (deposited on a SiO_2/p-doped Si heterostructure) by THz-TDS at room temperature, for $\omega/2\pi \in [0; \sim 8\ \mathrm{THz}]$, as a function of E_f. We controlled E_f (and hence the carrier density) by a gate voltage applied between graphene and doped Si. When graphene is substantially doped with E_f deep within the conduction or valence bands, $\tilde{\sigma}(\omega)$ follows the conventional Drude model, where intra-band transitions are predominant. Conversely, when graphene is neutral with E_f at the Dirac point, $\tilde{\sigma}(\omega)$ exhibits a very significant deviation from Drude-type models (i.e., Drude, Drude-Smith, Drude-Lorentz), with a notable suppression of its imaginary part $\mathrm{Im}[\tilde{\sigma}(\omega)]$.

We propose a two-component model based on the semiconductor Bloch equations which, by considering both intra- and inter-band electronic transitions, describes substantially better both the real and imaginary parts of $\tilde{\sigma}(\omega)$, $\mathrm{Re}[\tilde{\sigma}(\omega)]$ and $\mathrm{Im}[\tilde{\sigma}(\omega)]$, within a broad 0 - ~8 THz band, for a range of different E_f from doped to neutral graphene. In particular, this model explains the decrease of $\mathrm{Im}[\tilde{\sigma}(\omega)]$ observed for E_f near the charge neutrality point, as the result of an increase of interband contributions, which can be enhanced by structural deformations and electron-hole Coulomb coupling. Our findings highlight the non-Drude behavior of Dirac electrons in charge-neutral graphene, observable even at room temperature.

Structures and Phase Transitions at the start and end of the nuclear fuel cycle

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Uranium oxides are the foundation of the nuclear fuel cycle, presenting as complex chemical species in both uranium ore concentrates, to phases of interest in the development of stable waste forms at the end of the nuclear fuel cycle. Australia is a major exporter of uranium and has a responsibility to contribute to the long-term management of nuclear materials. This requires an in-depth structural understanding of materials present in the nuclear fuel cycle, and how they respond to changes in the environment.

Two such examples of uranium oxides at the start and end of the nuclear fuel cycle are $[UO_2(\eta^2\text{-}O_2)(H_2O)_2]$ (Metastudtite), and $CaUNb_2O_8$, a scheelite-type oxide.

The precise structure of Metastudtite is controversial with low resolution structural studies supported by DFT calculations suggesting that the trans-uranyl group is not linear. Non-linear uranyl groups are uncommon, with a recent study using Metastudtite sourced from the Beverley mine in Australia showing that the trans-uranyl groups are linear in conflict with the DFT study. We hope to resolve these issues using high resolution neutron diffraction to establish an accurate and precise structure of $[UO_2(\eta^2\text{-}O_2)(H_2O)_2]$ in a combined S-XRD+NPD study.

$CaUNb_2O_8$ is a rare example of a scheelite-type oxide containing U^{4+} on the 8-coordinate site. In situ variable temperature synchrotron X-ray powder diffraction confirmed a reversible phase transformation from fergusonite to scheelite. Paired with in situ neutron powder diffraction measurements, the nature of the fergusonite to scheelite transformation in $CaUNb_2O_8$ was revisited and the thermal stability of the scheelite explored.

Effective mass of polarons in perovskite materials

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Perovskite materials are used in a wide range of optoelectronic applications such as solar cells, light-emitting diodes (LEDs), LASERs, photo-rechargeable batteries, and radiation detectors.[1-5] There is the need to understand the structure and optoelectronic properties of these promising materials. The k•p method is very useful for providing analytical expressions to help gain insight into the band structure and physical phenomena occurring near the center of the Brillouin zone of semiconductor materials.[2] Analytical expressions for the effective mass of heavy, light, and split-off electrons are obtained by diagonalising the 8x8 k•p Hamiltonian.[3] For transport properties of charge carrier in highly polarizable semiconductors such as perovskite materials, polaron mass are of interest rather than the single-particle band effective mass.[4,5] The effective mass of polarons in perovskite is an indication of how effectively charge carriers are protected from scattering with longitudinal optical (LO) phonons.[4] Using the Frohlich's continuum theory of large polaron, we estimate the effective mass of polarons in perovskite semiconductors.

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Magnon dispersions in a Dresselhaus antiferromagnet

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Magnon spintronics, which focuses on the generation and manipulation of magnon, has been of considerable interest for application in computing devices. Magnon with nonreciprocal dispersions is attractive because it can be used to control the propagation of the magnon spin current. To obtain nonreciprocal dispersions, we can take advantage of the antisymmetric spin-exchange, Dzyaloshinskii–Moriya (DM) interaction in a noncentrosymmetric structure. The DM interaction shifts the bottom of the magnon dispersion away from the origin, which induces different group velocities for the magnon in the $+k$ and $-k$ directions, leading to the magnon propagation being nonreciprocal. It has been proposed in theory that a specific combination of DM interaction, easy-plane anisotropy Λ, and magnetic field brings the nonreciprocal magnon dispersion in Dresselhaus antiferromagnets [1]. $Ba_2MnGe_2O_7$ is a model compound with noncentrosymmetric space group $P\text{-}42_1m$. The magnetic moments align in *ab* plane with antiferromagnetic order below 4 K [2]. We thus measure magnon dispersions of $Ba_2MnGe_2O_7$ with external magnetic fields.

In this presentation, we will give results of inelastic neutron scattering for $Ba_2MnGe_2O_7$, taken on the cold neutron triple-axis spectrometer CG-4C CTAX at Oak Ridge National Laboratory, USA. The magnon dispersions are successfully observed, as shown in Fig 1. The comparison between magnon dispersions with applied horizontal magnetic fields along (0,1,0), (1,0,0), (1,-1,0) and linear spin-wave calculations will be presented.

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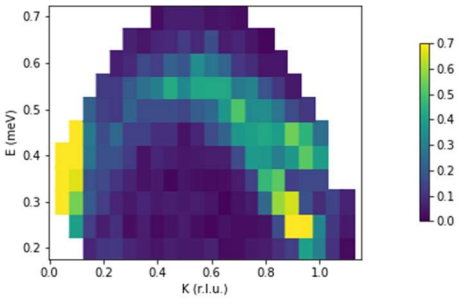

Fig1: Magnon dispersion measured at CG-4C CTAX in ORNL.

Effect of Ce doping on the structural and thermoelectric properties of $Bi_2Sr_2Co_2O_y$

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Thermoelectric materials convert thermal energy to electrical energy based on Seebeck effect [1,2]. Metal oxides are important thermoelectric materials due to their high thermal and chemical stability, tunable electrical and thermal properties, and well-established fabrication process along with relatively high thermoelectric performance [3]. In this work, $Bi_{2-x}Ce_xSr_2Co_2O_y$ ($0 \leq x \leq 0.15$) oxide-based samples were prepared by conventional solid-state reaction process. XRD patterns exhibited that the prepared samples had a monoclinic crystal structure and showed strong (0 0 l) diffraction peaks. SEM images showed a misfit-layered structure. The incorporation of Ce in $Bi_2Sr_2Co_2O_y$ slightly reduced the plate-like grain size. With increasing Ce concentration, the hole concentration decreased, whereas the hole mobility increased. The prepared samples showed a metallic conduction behavior. The incorporation of Ce in $Bi_2Sr_2Co_2O_y$ decreased the electrical conductivity due to the decrease in hole concentration. The Seebeck coefficients were very large due to the formation of layered superstructure. As the Ce concentration in the samples increased, the Seebeck coefficient increased due to the decrease in hole concentrations. The thermal conductivity decreased with increasing temperature, which was attributed to dominant phonon scattering at high temperatures. The figure-of-merit was enhanced with increasing temperature. In this study, the effect of Ce doping on the structural and thermoelectric properties of $Bi_{2-x}Ce_xSr_2Co_2O_y$ was systematically investigated.

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Investigating the Anharmonic Collapse of Phonon Dispersions in Thermoelectric Chalcogenides

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Thermoelectrics operate by the thermoelectric effect where a current is produced by applying heat to a junction and can also operate conversely as a refrigerant by the application of a current to produce a heat gradient [1]. Appropriate materials for use as a thermoelectric are those with low thermal conductivity and a high thermoelectric power factor. To optimize thermoelectric efficiency, phonon relaxation times can be decreased by the introduction of defects and/or increasing phonon anharmonicity [2]. Recently, a superb thermoelectric performance was measured in SnSe, attributed to its unique phonon characteristics. In particular, the softening of phonon modes induced by a temperature dependent structural transition generates a giant phonon anharmonicity [3] [4].

This work presents preliminary studies of phonon modes in SnSe measured through inelastic time-of-flight neutron spectroscopy which reveals large anharmonicity and evidence of phonon softening. Density functional theory calculations through VASP and nMoldyn were performed to model the geometry, frequencies, and intensities of SnSe phonon modes. These calculations correctly predict phonon energies in SnSe time-of-flight data and reinforce the observations of phonon softening.

The findings of this work demonstrate mechanisms that could be used to increase phonon anharmonicity and will be a useful guide for future work in thermoelectric materials.

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Braiding of Majorana zero modes

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Majorana zero modes are quasiparticles which can be found as "mid-gap states" in topological superconductors. Qubits consisting of Majorana zero modes are the primary path towards topologically protected quantum computing. There is growing evidence that Majorana zero modes have been realized in solid-state experiments, and also the number of different platforms is growing. Today first braiding experiments are under way, and it is thus timely to challenge our understanding of how a topological quantum computer would work. In particular, it is crucial to understand how braiding errors can be introduced from sources such as quasiparticle poisoning, Majorana hybridization, and diabatic processes. It is not fully understood how these error rates behave in a full quasiparticle background, which is often included using the full exponential Hilbert space.

That is, one needs to investigate the time-evolved many-body states describing a topological superconductor hosting several Majorana zero modes. We present a method to calculate expectation values and overlaps of time evolved many-body states from single-particle states in a superconductor [1]. We calculate the fidelity, transition probabilities, and joint parities of Majorana pairs to quantify the braiding errors. We show how error rates depend on the timescale and smoothness of the time dependence, as well as the energy gap and distance between Majorana zero modes. This method is a powerful tool to test and analyze the many theoretical implementations of Majorana qubits. Moreover, this method can be used to study the dynamics of any superconducting system.

We acknowledge financial support from the Australian Research Council through Grant No. DP200101118.

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Data processing technique for the Taipan "Be-filter" neutron spectrometer at ANSTO

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Taipan, the highest flux thermal neutron scattering instrument at ACNS, was originally built as a traditional triple-axis spectrometer. In 2016 a beryllium filter analyser spectrometer was added for increased versatility. The Be-filter acts like a low-energy band-pass filter ideal for investigating lattice dynamics and molecular vibrations over a wide energy range. It is particularly well suited to measuring the motion within materials containing light elements such as hydrogen.

We have successfully created a robust method of treating data from the Taipan filter-analyser and present the method within this poster [1]. The data-treatment process includes correction for the non-linear energy variation of a particular monochromator, removal of higher-order wavelength contamination, and estimation of low-energy multiple-scattering. The steps described here can be utilized by all users of the Australian Nuclear Science and Technology Organisation "Be-filter"—past, present, and future.

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DFT Generated Scattering Factors for IAM in QCBED in light metal alloy determinations

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Quantitative Convergent Beam Election Diffraction (QCBED) has become a well-established experimental method providing unique insights into such phenomena as electron bonding and material strength [1]. This method relies on the input of electron scattering factors into the computational analysis of the electron scattering process within the crystalline material, whether by Bloch wave or multi-slice formulation.

Analysis of the electron bonding within materials is made by comparison to the electron scattering factors from an Independent Atom Model (IAM) - with atoms no longer on a finite crystalline lattice, but instead notionally infinitely distant from one another [2]. Standard values of the electron scattering factors for electron microscopy use Fourier transforms of Hartree Fock (HF) computations for the atomic electron charge density and associated potential. However, HF does not include all electron correlation effects that might introduce real space charge redistribution, with associated changes in scattering angle s dependency.
Difficulties in calculation of the electron scattering factor associated with the potential have been recognized especially for small s values and accordingly the Mott - Bethe formula is most often used to convert results from the more numerically stable X-ray scattering factor. Instead, this work addresses these issues directly by modifying slightly the Density Functional Theory (DFT) computational package WIEN2k that employs a combination of augmented plane waves with local atomic orbitals. This is possible because its iterative structure explicitly uses the Poisson equation (and hence Mott-Bethe formula) to directly tie together at each iteration the electron density with the potential.

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‘Wagga’ Tribute to Timothy John Bastow

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Notwithstanding that Timothy John Bastow may have started life as an infant without a deep knowledge of condensed matter physics, he soon turned his curiosity and love of nature’s ways into a brilliant career in physics. Tim gained his B.Sc. in Physics (1957 – 1960) at The University of Melbourne and PhD in Physics (1961 – 1966) at Monash University studying the magnetic structure and properties of chromium and dilute chromium alloys, supervised by Professor R. Street. He held a Science Research Council Fellowship (1966 – 1970) at the University of Cambridge, Cavendish Laboratory, working on the topic of laser interactions with solid surfaces and surface thermal expansion with Professor F. P. Bowden. At Cambridge he also worked with Professor D. Tabor. Tim’s astute papers from these early days on pure chromium, dilute chromium alloys, and chromium surface properties are still receiving citations.

Tim Bastow *c.* 1940

Tim came back to Australia to join CSIRO in 1970. He became a Senior Principal Research Scientist and leader of the solid state nuclear magnetic resonance (NMR) group, retiring in December 2014 to become an Honorary Fellow through 2021, and spending most of his career working in the building named for his father (Stewart Bastow Laboratory). To date, there have only been 6 years in CSIRO’s history without Tim or his father at work there!

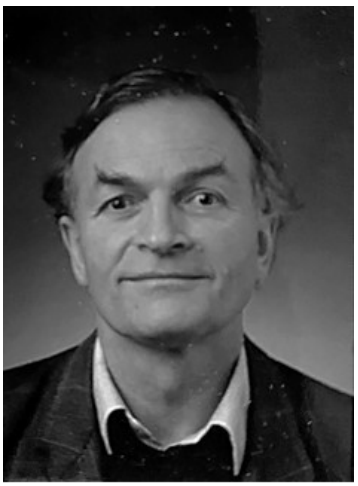
Tim Bastow *c.* 1970

Tim’s scientific passion was zero-field NMR which is where he started his CSIRO career and where he returned in recent years. Tim established nuclear quadrupole resonance (NQR) and NMR as multi-nuclear solid state analytical techniques at CSIRO. He discovered a new class of antiferromagnetic CuII compounds and a new class of electrically ordered compounds. He discovered that natural abundance ^{17}O NMR could be obtained in many metal oxides by the magic angle spinning technique, and he discovered that spectroscopic signatures of alloy precipitate phases were clearly and unmistakably observable in the NMR spectra of the probe atomic nucleus.

His published works are here: https://publons.com/researcher/2655868/timothy-j-bastow/.

Tim’s research publications total 174 journal papers, 4 book chapters, and 8 crystallography open database entries garnering, at writing of this abstract in early December 2021, greater than 4500 citations and an h-index of 35 according to Web of Science. Tim was twice awarded a CSIRO Medal for Research Achievement and twice shortlisted for the Australian Academy of Science Lyle Medal for Physics and Mathematics. He accepted invitations to deliver over 40 invited and plenary lectures. He was awarded a Leverhulme Trust Professorship at The University of Warwick in 2004 and an Honorary Professorship at Deakin University in 2011.

Tim's sustained contributions to CSIRO's impact span his career and include underpinning several CSIRO patent families using ^{27}Al NMR for reactive aluminas; ^{89}Y NMR for quality-controlled processing of high-Tc superconducting ceramics; ^{91}Zr for zirconia-based electrolyte processing; ^{63}Cu, ^{25}Mg, ^{27}Al, and ^{45}Sc for secondary aging of industrial aluminium alloys; and ^{75}As and ^{63}Cu for rapid on-line NQR detection of minerals and compounds.



Tim Bastow *c.* 1990

For his friends and colleagues, his greatest contributions were his generous mentorship and infectious love of scientific discovery which made working with him a joy.

Tim was a long-time attendee and supporter of 'Wagga' from his first conference attendance in 1979. Tim contributed papers to twenty 'Wagga' conferences over the years, and he was a co-organiser and chair of 'Wagga' in 1983, 1990, and 2009.

Tim loved physics and mathematics puzzles and constructed numerous working examples of wonder for his friends and family, some of which will be shown in the presentation. The presentation will cover some highlights of Tim's career with quotes from some of his collaborators.

Gold-Manganese: Phase Transformations and Diffusion Studies

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In recent years antiferromagnetic spintronics has become a field of interest with respect to memory storage devices. As a result there has been a renewed interest in the study of ordered antiferromagnetic materials. One such system is Au-Mn. There is still much to learn about Au-Mn alloys and, for example, the binary phase diagram is not entirely settled yet. It is known, however, that there are several antiferromagnetic phases in the Au-Mn system. In our work we have focused on AuMn and $AuMn_2$. The former is interesting because it has a wide range of compositional stability on either side of the equiatomic ratio and because it undergoes solid-state transformations below 200 °C that could potentially be used to switch the antiferromagnetic property on or off. In contrast, $AuMn_2$ is a line compound and is reported to be stable in its antiferromagnetic form to 680 °C. Here we discuss the Au-Mn systems and present synchrotron X-ray diffraction results showing the phase transformations with change in temperature for $Au_{51.5}Mn_{48.5}$ and initial results for diffusion studies on Au-Mn-Au trilayer systems studied using X-ray reflectometry. In the latter case the objective is to investigate whether high quality antiferromagnetic thin films can be grown in situ by solid state reactions.

Phonon Engineering Tin Telluride Guided by Inelastic Neutron Scattering

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The challenge of designing a highly performing thermoelectric material lies in the requirement to de-couple the electronic and thermal transport; creating a material that has the electronic properties of a highly conducting crystal, while simultaneously having the thermal properties of a poorly conducting glass. The phonon-glass electron-crystal concept has contributed to significant research on the "phonon engineering" of materials. One exceptionally useful tool for aiding this engineering process is inelastic neutron scattering (INS). Information such as phonon linewidth, dispersion, and density of states (DOS), directly obtained by INS, can all be related back to the thermal properties of materials. In this talk, I will give an overview of the usefulness of INS as a tool to study phonons in thermoelectric materials by presenting some of our recent INS data on chalcogenide-based thermoelectric materials obtained at the Australian Centre for Neutron Scattering. In our work, we explore how INS can be used to understand the thermal conductivity of SnTe by studying the evolution of phonon modes as a function of temperature using Pelican (time-of-flight), Sika and Taipan (triple-axis). We also compare data obtained by each instrument and highlight significant and unexpected differences. We observe clear acoustic phonons, together with a highly dispersive anomalous optical phonons, which broaden with temperature as the phonon-scattering rate increases. Additionally, we study the phonon DOS of carbon nanomaterials, such as nanodiamond, to understand their intrinsic phonon lattice dynamics, and compare them with thermoelectrics to understand phonon scattering in nanocarbon doped thermoelectric composites due to thermal boundary resistance. We observe extremely broadened phonon modes in the nanoparticles compared to their bulk counterparts, and little overlap in the density of states when compared to thermoelectric materials.

Neutron Ray Tracing Calculations of Taipan, a Thermal Neutron Triple-Axis Spectrometer

L. Covey, R. Stockton, and A.P.J. Stampfl

Australian Nuclear Science and Technology Organisation.

McStas is a well-known ray-tracing program for the design, development, investigation of neutron instruments as well as a potential learning and teaching tool for those that wish to understand or show how a neutron instrument works.

Here we build the thermal neutron triple-axis spectrometer on Taipan in McStas, configuring it to determine the resolution function in R(,Q) under a number of different configurations. We are initially interested in how the lengths of the arms of the triple-axis alter the resolution function, in-particular how close we can place the analyser to the sample before losing usable resolution. We are wishing to potentially increase scattered flux without degrading resolution. We also wish to explore how reducing the thickness of the sapphire filter in the pre-optics affects the ultimate resolution of the spectrometer. We discuss our results to-date.

This study is the result of a Macquarie University PACE (Professional and Community Engagement) program where third/fourth year Physics students work for three weeks with a company or government institution on a research, development, or industry project.

On the Metastability of $CsPbI_3$ Perovskite and How to Fix It

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A new generation of semiconducting materials based on metal halide perovskites has been launched into the scientific spotlight, exhibiting outstanding optoelectronic properties and providing promise for the development of efficient optical devices [1]. As a vivid example, solar cells made from these materials have quickly reached conversion efficiencies on par with well-established technologies, like silicon. Their widespread success is due, in part, to a unique ability to retain high-quality optoelectronic performance while being easily solution-processed into thin films. However, the interesting photophysics of metal halide perovskites come with a catch; their soft ionic structure promotes complex thermal-induced phase transitions and a variety of dynamic structural behavior. Such properties have ultimately made understanding several important structure–property relationships ambiguous and obstructed a clear technological path due to inherent phase instability [2].

Our aim in this contribution is to highlight the fundamental aspects of metal halide perovskites that dictate a stable crystal structure, through the lens of thermodynamic preference and phase formation energies [3]. Taking the all-inorganic $CsPbI_3$ system as a suitable case study, we focus on several ways in which its thermodynamically unstable perovskite structure can be maintained at room temperature and elucidate the restructuring pathways taken during destabilization. In addition, we will discuss the origin and mechanisms of phase decay within real-world devices, with emphasis made toward direct visualization using advanced in situ techniques and arriving at quantitative results. For several notable features of halide perovskites dealt with in this contribution, e.g., strain [4,5] and compositional stabilization [6], environmental phase triggers [7], nonperovskite phase restructuring pathway [3], and lattice anchoring [8], we attempt to rationalize them using state-of-the-art materials modeling techniques.

It is within this spirit that we not only modify a broad range of properties existing within metal halide perovskites, but regulate them for enhanced functionality. We anticipate that providing a clear perspective for these topics will help deepen our knowledge of the nature of ionic semiconductors in general, and provide the stimulus required to build new research directions toward harnessing metastable phases of promising optoelectronic materials.

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A Mössbauer investigation of potential electrode candidates

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The research reported here is part of a larger project directed at potential electrode candidates based on iron-based salts; some of which are common pharmaceutical salts. A series of such Fe-containing compounds, some synthesized in-house while others purchased, have been examined as electrodes in lithium-ion batteries. These electrodes show exceptional electrochemical performance [1] but their mechanism is not fully understood.

We report here on initial Mössbauer spectroscopy characterisations of the pristine materials that are designed to pave the way for the analysis of more complex electrochemically cycled samples. Mössbauer spectroscopy provides useful site environment information from the quadrupole splitting parameter and the Fe valence state is determined from the isomer shift parameter.

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Skyrmion nucleation on the surface of a topological insulator

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Skyrmion nucleation induced by spin-transfer torques at an interface of a topological insulator and a ferromagnetic insulator is investigated. Due to strong spin-orbit coupling on a surface of topological insulators, which enhances the effect of spin torques, efficient manipulation of skyrmions is expected and therefore, topological insulators could provide the ideal platform to achieve high-performance skyrmionic devices. Using micromagnetic simulations and energetics, we evaluate properties of the skyrmion nucleation on a surface of topological insulators, such as nucleation time, critical electric field, and skyrmion numbers [1]. We show that the nucleation time is inversely proportional to the applied electric field. We also identify the Gilbert damping and temperature dependences of the critical field. Furthermore, we analytically evaluate the effect of the Dzyaloshinskii-Moriya interaction and demonstrate that the temperature dependence can be explained by the reduction of a magnon excitation gap due to the self-energy corrections.

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Scaling Behaviour and Stability of Magnetic Skyrmions in Cu_2OSeO_3

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A skyrmion is a topological stable particle-like object comparable to spin vortex at the nanometre scale. It consists of an about 50 nm large spin rotation which order in a 2 dimensional, typically hexagonal superstructure perpendicular to an applied external magnetic field. Its dynamics has links to flux line vortices as in high temperature superconductors. Cu_2OSeO_3 is a unique case of a multiferroic materials where the skyrmion dynamics could be controlled through the application of an external electric field. The direct control of the skyrmion dynamics through a non-dissipative method would offer technological benefits.

Important for technological applications would be a stability range of the skyrmion phase up to room temperature. While room temperature skyrmion materials exist, Cu_2OSeO_3 orders magnetically below 60 K. Our combined small angle neutron scattering and SQUID magnetization measurements did provide direct evidence that the stability range of the skyrmion phase can be extended in Te-doped Cu_2OSeO_3. Besides the information about the skyrmion range in the H-T phase diagram, neutron scattering provides also the full information about the orientation and skyrmion distances in the skyrmion lattice. Our systematic investigation offers new aspects about the scaling behaviour of the skyrmion and helical distances as a function of temperature and magnetic field. It is interesting to note that the changes in skyrmion distances are quite distinct for the different skyrmion phases, observed for different crystal orientations. The results provide new valuable information on the parameters in the spin Hamiltonian, which are responsible for the formation of the fascination quantum protected objects.

Reduced crystal symmetry as the origin of the ferroelectric polarization within the incommensurate magnetic phase of $TbMn_2O_5$

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The precise crystal symmetry and hence the emergence of the electric polarization still remains an open question in the multiferroic material RMn_2O_5 (R = rare-earth, Bi, Y). While previous diffraction studies have indicated that RMn_2O_5 possesses the centro-symmetric space group P*bam*, an atomic displacement allowing for the electric polarization would require a non-centrosymmetric crystal symmetry.

Our single crystal neutron diffraction experiments on $TbMn_2O_5$ provide direct evidence of a reduced crystallographic symmetry already above the magnetic and ferroelectric phase transitions and a change in magnetic order upon entering the ferroelectric phase [1]. This is indicated through the presence of additional nuclear Bragg peaks that are forbidden for the space group P*bam* but are in good agreement with the polar space group P12_11. It implies that the exchange-striction, which arises from a symmetric $\mathbf{S_i} \cdot \mathbf{S_j}$ spin coupling, is the dominating mechanism for the generation of the electric polarization in the commensurate magnetic phase of $TbMn_2O_5$. Furthermore, the commensurate magnetic reflections are in accordance with a quartile step spin-spiral along the c-axis. Therefore, the antisymmetric $\mathbf{S_i} \times \mathbf{S_j}$ exchange via the inverse Dzyaloshinskii-Moriya interaction contributes as well and becomes the leading term in the low temperature incommensurate spin-spiral magnetic phase. These new findings provide important information for the understanding of the complex interplay between the magnetic and the structural order throughout the RMn_2O_5 series of multiferroics.

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Structural anomaly upon Te-doping in the magnetic transition regions of insulating helimagnet $Cu_2OSe_{1-y}Te_yO_3$

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Unconventional topological in-chiral spin systems offer a plethora of fascinating phenomena for fundamental research and future technological applications.[1] There are key structural criterions for the formation of such textures, these include a compatible structure with suitable topology, along with an underlying mechanism that stabilises the resulting spin texture. Chiral magnets with broken inversion symmetry where competing Heisenberg and Dzyaloshinskii–Moriya (DM) interactions favour twisted spin structures with λ = 10–200 nm can host magnetic skyrmions lattice (SkL).[2] Due to the complex spin and charge interactions in these systems, the underlying processes leading to the ordering are still not fully understood. Cu_2OSeO_3 is an insulating multiferroic material that has shown to host SkL at specific conditions.[3] It possesses a magnetic structure with both ferromagnetic (FM) and antiferromagnetic (AFM) super exchange interactions being present and has a 3-up 1-down ferrimagnetic arrangement of Cu^{2+} ions.[4] The lack of inversion symmetry in the corner shared O-Cu_4 tetrahedra lattice results in an appreciable DMI between Cu^{2+} sites; this competes with FM/AFM interactions leading to spin canting formation of helical/conical spin textures at different fields and temperature conditions.[3] Due to the absence of changes in the crystal structure throughout the temperature range alongside the formation of the magnetic phases, it has been commonly assumed that the structure plays a passive role in the transition between magnetic phases.[4] However, low temperature single crystal XRD data we measured indicated an anomalous trend in Cu-Cu bond distances over the temperature range matching the different magnetic ordering. This was observed by Dutta *et al.* during cooling in their polycrystalline samples and further indicated the inverse trends in the Cu-Cu distances between the 'strongly' and 'weakly' interacting O-Cu_4 tetrahedra.[5] Furthermore, observation by Nishibori *et al.* shows that by applying a pressure, T_c increases as the unit cell volume contracts.[6] This further supports the role crystal distortion has on the magnetic phases.

The project's focus is on the relationship between the crystal structure and magnetic ordering observed in the Cu_2OSeO_3 material system upon substitution in the Se non-magnetic sites with Te. As the ionic radii of Te^{4+} and Se^{4+} ions are 140 pm and 107 pm, respectively, incorporation of the much bigger Te^{4+} ion into the Se site would result in an expansion of the crystal structure without changing the magnetic contributions from Cu^{2+}. A series of $Cu_2OSe_{1-x}Te_xO_3$ with x up to 0.15 were synthesised. Using both neutron and synchrotron X-ray powder diffraction, and magnetisation measurements, we show a link between structural distortion and the formation of the magnetic phases present in the Cu_2OSeO_3 material system.

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Asymmetric antibimerons: statics and dynamics

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The non-trivial topological spin textures, such as magnetic skyrmions, have been of great interest recently due to their potential use as information carriers in spintronic memories. In this work we theoretically predict an existence of an asymmetric antibimeron - a novel topological texture in in-plane magnetized chiral ferromagnet with D_{2d} symmetry, which is yet to be observed experimentally. We show that it can be stabilized by the anisotropic interfacial Dzyaloshinskii-Moriya interaction, which is found in materials with D_{2d} symmetry. Using energetic considerations, we explain its asymmetric shape formed of an antivortex and a crescent-shaped vortex of opposite core polarizations. Furthermore, we demonstrate that asymmetric antibimerons of opposite topological charge can be stabilized within the same ferromagnetic film, unlike skyrmions in out-of-plane magnetized films. Employing micromagnetic simulations, we also investigate stability and current-driven dynamics of the asymmetric antibimerons, as well as their collisions. Our results shed light on a fundamental understanding of asymmetric topological magnetic solitons and provide guidance for their experimental observation in in-plane magnetized ferromagnets.

Visualization of Strain-Induced Landau Levels in a Graphene - Black Phosphorus Heterostructure

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Graphene, with its linear band dispersion at low energy and massless Dirac-like fermions, allows the Quantum Hall effect (QHE) to be observed at room temperature under a strong magnetic field[1]. In the QHE, electrons will travel in quantized cyclotron orbits with discrete energy levels called Landau levels (LLs). Yet, the massless Dirac-like behaviour of graphene provides a potential avenue to realise LLs without the need for strong magnetic fields as it allows electronic band structure modification by lattice deformation. If a non-uniform distortion is applied to the graphene lattice it shifts the graphene Dirac cones at K and K' in two opposite directions and thus generates a pseudo magnetic field (PMF)[2]. Strain induced pseudo magnetic fields offer the possibility of generating zero magnetic field Quantum Hall effect in graphene, possibly up to room temperature. Strain engineering on graphene is usually achieved via random nanobubbles or artificial nanostructures on the substrate[3,4]. Heterostructure engineering offers an alternative approach, by stacking graphene on another van der Waals material with large lattice mismatch at a desired twist angle it is possible to generate large strain induced pseudo magnetic fields over the entire heterostructure[5].

In this study, we used nano-angle resolved photoemission spectroscopy (nano-ARPES) to probe the electronic bandstructure of a graphene - black phosphorus heterostructure. ARPES is a momentum and energy resolved technique that has proven to be a powerful tool in directly studying the electronic bandstructure of 2D materials and heterostructures. By directly measuring the iso-energy contours of graphene and black phosphorus we determine our heterostructure has a twist angle of 20-degrees. This twist angle, together with the large lattice mismatch between graphene and black phosphorus creates a shear strained superlattice which gives rise to a periodic PMF across the entire heterostructure. High-resolution nano-ARPES of the graphene bands near the Fermi level reveals a large increase in the Fermi velocity and the emergence of flat bands located within the Dirac cone. The spacing of the flat bands is consistent with Landau level formation in graphene, and corresponds to a pseudo-field of 10 T. Our work provides a new way to study quantum Hall phases induced by strain in 2D materials and heterostructures.

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Multidimensional Ramsey Spectroscopy of Impurities in Ultracold Fermi Gases

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Polaron, arguably the most celebrated quasiparticle, consists of an impurity dressed with elementary excitations of a many-body background. Polaron plays an essential role in understanding the properties of a wide variety of quantum materials, such as monolayer transition metal dichalcogenides. Ultracold gases provide a perfect experimental platform for investigating the associated impurity problem, thanks to the unprecedented controllability and rich atomic physics toolbox.

Ramsey spectroscopy is one of these established techniques in ultracold gases. It is similar to the renowned nuclear magnetic resonance (NMR) interferometry, which manipulates internal (e.g., pseudospin instead of spin) degrees of freedom and observes the interference determined by the surrounding many-body environment. Conventional Ramsey spectroscopy usually shows the signal as a function of one single variable, and hence called one-dimensional (1D). Our recent studies push the well-established 1D Ramsey spectroscopy into multidimensional (MD). This new tool allows observation of nonlinear nonequilibrium dynamics of an impurity in ultracold Fermi gases manipulated by a series of radiofrequency (RF) pulses at several different times and reveals many-body correlations unfolded in conventional 1D spectroscopy.

For the case of a heavy impurity [1], we perform an in-principal exact calculation via the functional determinant approach [2,3]. On the other hand, for the case of a mobile impurity, we obtain an exact analytic expression using Chevy's ansatz. Our results show a strong correlation between attractive and repulsive Fermi polarons, evidenced by the two off-diagonal cross-peaks in the two-dimensional spectrum. We also observe the many-body coherent and relaxation dynamics of the system as quantum beats between the cross-peaks. Our scheme provides a new method to investigate many-body nonequilibrium physics beyond the linear response regime with the accessible tools in cold atoms. Our method can also be regarded as a cold-atom analogue of the 2D coherent spectroscopy (2DCS) in solid state physics, where the relation and differences between MD Ramsey spectroscopy of Fermi polaron and 2DCS of exciton-polaron in monolayer transition metal dichalcogenides will be discussed.

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Observation of new level crossings and strong electron-hole asymmetry in the Landau Octet of bilayer graphene

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Bilayer graphene consists of two layers of honeycomb carbon lattices. Its zero energy Landau level, the lowest quantized energy of the cyclotron motion of charged particles in a uniform magnetic field, is nearly 8-fold degenerate, due to its spin (σ), valley (ξ), and orbital (N) symmetries. In the presence of magnetic fields and electric fields, the 8-fold degeneracy can be lifted, which could result in complex symmetry breaking states $|\sigma, \xi, N>$ in terms of different combination of spin (σ), valley (ξ), and orbital (N) quantum numbers. Furthermore, multiple energy level crossings are observed between different symmetry breaking states as electric fields are varied. The multiple symmetry breaking states of the zero-energy Landau level, combining with its electrical tunability, makes bilayer graphene an attractive platform for engineering exotic quantum states [1-6]. Therefore, determining symmetry breaking states at different electric fields which these exotic quantum states are based on is essential, but is found very challenging. So far this can only be done by certain capacitance measurements [7,8], but not by transport measurements.

In this work we present transport measurements of zero-energy Landau level spectra of a BLG device in much larger electric fields than reported previously. We observe new zero-energy Landau level crossings in high electric fields, which exhibit strong electron-hole asymmetry. The new observations provide constrains on fitting parameters in the modelling and enable us to determine the complete phase diagram of symmetry breaking states at different magnetic fields and electric fields. Our work paves the way of using transport measurements for understanding and engineering the zero-energy Landau level of BLG for exotic quantum states.

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The origin of spin reorientation in the 2D triangular antiferromagnet.

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A two-dimensional (2D) triangular lattice Heisenberg antiferromagnet (2D-THA) is one of the simplest examples of geometrically frustrated antiferromagnets. A novel spin state originated from low dimensionality and competing for magnetic interaction is expected. The materials of interest in this study are (Lu, Y)MnO_3 and (Lu, Sc)FeO_3. Both have P63cm symmetry and 120 degrees antiferromagnetic structures but the exchange interactions in nearest neighbors are $J \sim 2.5$ meV with $S = 2$ (Mn^{3+}) and $J \sim 4.0$ meV with $S = 5/2$ (Fe^{3+}). We have made a systematic investigation of polycrystalline and single-crystal samples by using neutron diffraction, inelastic scattering, and polarized neutron scattering experiments to understand the 2D-THA system. We focus on these three results in this presentation

1. The development of determining the magnetic structure of 2D-THAs
2. The origin of the spin reorientation observed in the 2D-THAs
3. A classical spin liquid state or extended critical range observed in the 2D-THAs

Four possible 120-degree antiferromagnetic structures are Γ_1, Γ_2, Γ_3 or Γ_4 in this P63cm symmetry. They cannot be distinguished using unpolarised neutron scattering techniques. By using both polarized neutron scattering techniques, we developed techniques to solve it uniquely. For example, the magnetic structures of $Lu_{0.3}Y_{0.7}MnO_3$ and $Lu_{0.47}Sc_{0.52}FeO_3$ are determined as $C_1\Gamma_3 + C_2\Gamma_4$ and $C_3\Gamma_1 + C_4\Gamma_2$ respectively. To understand the spin reorientation often observed in 2D-THA, we have measured magnon dispersions of $Lu_{0.3}Y_{0.7}MnO_3$ and $Lu_{0.47}Sc_{0.52}FeO_3$ and analyzed based on the Hamiltonian below,

$$H = \sum_{<i,j>} J_{ij}\,\vec{S}_i \cdot \vec{S}_j - D_1 \sum_i (S_i^z)^2 - D_2 \sum_i \left(\vec{S}_i \cdot \vec{n}_i\right)^2.$$

J_1 and J_2 are exchange parameters between Mn atoms in-plane, and J_{1z} and J_{2z} are exchange parameters between Mn atoms along the c-axis. D_1 is in-plane anisotropy and D_2 is out-of-plane anisotropy. The overall magnon dispersion looks similar because both have P63cm and 120-degree antiferromagnetic structures. We found interactions interlayer are important to understand the spin reorientations. Finally, we are interested in diffusive magnetic excitation observed in both $Lu_{0.3}Y_{0.7}MnO_3$ and $Lu_{0.47}Sc_{0.52}FeO_3$ just above T_N shown in the Figure. The phenomena are widely observed in the 2D-THA, and we are trying to model them.

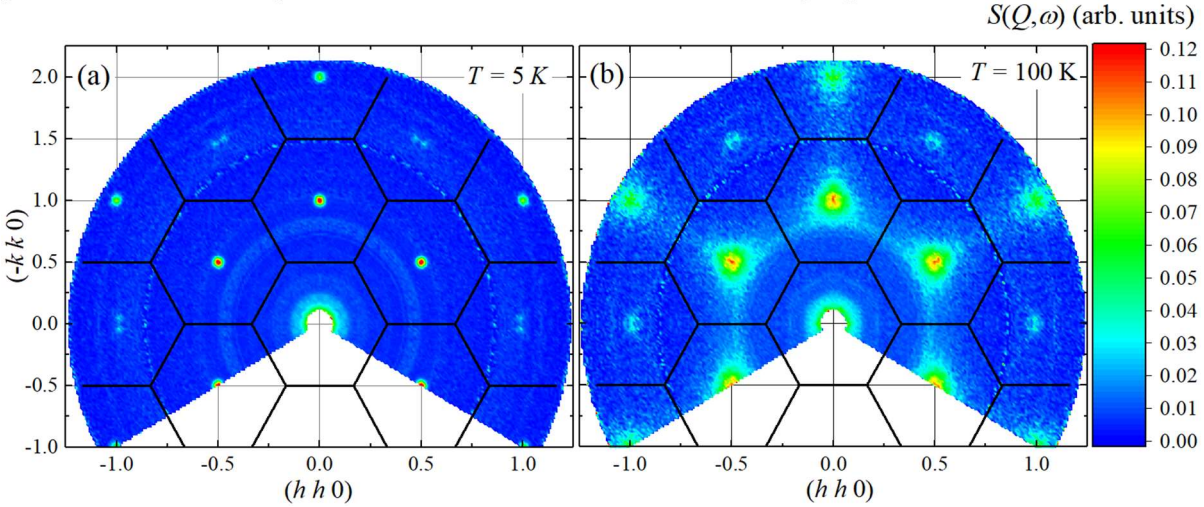

Figure 1. The contour map of $S(Q,\omega)$ was taken at 5 K and 100 K on HRC J-PARC.

Temperature-dependent structural anomaly in the magnetic transition regions of insulating helimagnet Cu_2OSeO_3

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Magnetic skyrmions lattice (SkL) is a periodic array of vortex-like spin textures which are protected against decay due to their non-trivial topology. Their particle-like nature and topological protection makes them fascinating candidates for both fundamental research and future spintronic devices. Cu_2OSeO_3 is an insulating magnet which crystallises into the cubic non-centrosymmetric space group $P2_13$. Due to the lack of an inversion symmetry, competing Heisenberg and Dzyaloshinskii–Moriya (DM) interactions leads to a helical spin ordering below T_c [1]. Upon the application of a magnetic field, the helical phase can further modulate into other magnetic orderings including conical, ferrimagnetic, and SkL [2]. Commonly, the corner sharing distorted Cu_4-tetrahedra (along the body diagonal) with two crystallographically distinct Cu^{2+} ion sites is offered as the basis for the magnetism [3]. While it has been accepted that no crystallographic transformation accompanies the transition between the paramagnetic and helical phases [3], recent work by Dutta *et al.* has shown a temperature dependent change to the distortion of the Cu_1-Cu_2 distance between the 'strongly' and 'weakly' interacting O-Cu_4 tetrahedra (with the distance decreasing and increasing respectively) over that region [4].
Here, we propose an addition to the conventional Cu_4-tetrahedral model by considering the Cu^{2+} site as being in a 3D Kagome lattice, such that a network of triangular lattice connects the magnetic ions. Through a range of temperature depending structural characterisation techniques including single crystal XRD, synchrotron powder XRD, and neutron powder diffraction data, we show in detail the temperature dependent structural anomaly of Cu_2OSeO_3 over the range of magnetic phase transition. From this, we observed a systematic distortion to the Kagome lattice which occurs concurrently with magnetic phase transition. The work presented provide insight highlighting the role structure may be playing in causing the magnetic ordering of this magnetic system.

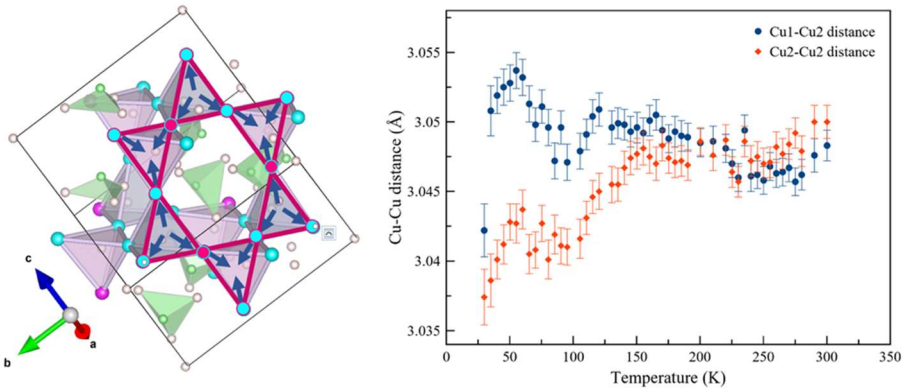

Figure 1 The Kagome motif of Cu_2OSeO_3 and the temperature dependent changes to the Cu-Cu distance as determined by SC XRD

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PELICAN –a Time of Flight Cold Neutron Spectrometer – Recent Scientific Outcomes and New Capabilities

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The time-of-flight direct-geometry neutron spectrometer, Pelican, has been in user program since 2014 at the OPAL research reactor, at the Australian Nuclear Science and Technology Organisation (ANSTO) [1]. The Pelican instrument was designed to meet the diverse requirements of the Australian scientific community from physics, chemistry, material science, to biology. A wide range of research fields is covered. These include crystal-field excitations, phonon densities of states, magnetic excitations for various multifunctional materials including high Tc superconductors, novel magnetic, thermoelectric, ferroelectric and piezoelectric materials; molecular dynamics in hydrogen-bonded and storage materials, catalytic materials, cements, soils and rocks; and water dynamics in proteins and ion diffusion in membranes. Polarized neutrons and polarisation analysis option makes the full use of the neutron spin to study magnetism and to separate the coherent and incoherent scatterings.

In this presentation, the recent scientific outcomes and recent developments of new capabilities of the instrument will be demonstrated with several systems studied using quasi-elastic and inelastic neutron scatterings. These include water dynamics around amino acids, crystal field excitations in magnetic molecular crystals, low energy magnetic excitations in spin frustrated magnet, oxygen diffusion in solid oxide conductors and phonon density of states in energy materials. To meet the demand of diverse user community, new sample environment equipment has been developed and commissioned including high pressure cell, in-situ light irradiation, fast dilution temperature cooling system and superconducting magnet. These new developments have significantly extended the instrument capabilities.

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Roles of Anharmonic Lattice Dynamics and Fast Magnetic Fluctuations Played in Advanced Caloric Materials – a Study with Inelastic Neutron Scatterings

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Refrigeration is of vital importance for modern society—for example, for food storage and air conditioning—and 25 to 30 per cent of the world's electricity is consumed for refrigeration. Current refrigeration technology, mostly involving the conventional vapour compression cycle, is of growing environmental concern because of large amount of greenhouse gases released into atmosphere every year. As a promising alternative, refrigeration technologies based on solid-state caloric effects have been attracting attention for several decades. Searching for novel materials having large isothermal entropy changes upon phase transition induced by a small external field is the core activity in the study of solid-state caloric effects. To understand the mechanism of the large caloric effect and the associated phase transition is fundamentally important. In this presentation, I will report how inelastic neutron scattering and quasi-elastic neutron scattering can reveal the mechanism responsible for the colossal barocaloric effects (CBCEs) (large cooling effects induced by pressure) from plastic crystals [1] and the role of fast magnetic fluctuations played in the first order phase transition of the giant magnetocaloric material $LaFe_{11.6}Si_{1.4}$ [2].

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Observation of Magnetic Peaks in Half-Metallic Sr_2CrMoO_6

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Half metal is a special metallic material with 100% spin polarization; that is, all the electrons at the Fermi Level in the half metal are either spin up or spin down. The characteristic has major implications for the efficiency of spintronic devices such as giant magnetoresistance (GMR), tunnelling magnetoresistance (TMR) devices. The double perovskite structure Sr_2CrMoO_6 (SCMO) is a ferrimagnet, with antiparallel coupling between Cr^{3+} and Mo^{5+} moments below its ordering temperature ~473 K.[1] Theoretical calculations[2-4] predicted that the density of states near the Fermi level are fully contributed by the Mo's 4d electrons, which are fully spin polarized. As an electronic material, the SCMO thin film possesses ultrahigh mobility[2], e.g., ~ 10000 cm^2/Vs, which could minimize the dissipation in electronic devices. To study the magnetic structure in the SCMO thin film (1 μm thickness on *a*-oriented $SrTiO_3$ substrate, SCMO sample mass ~ 0.5 mg), the triple axis neutron spectrometer Taipan was employed to seek for the magnetic peak. The thin film was mount in *HHL* scattering plane during the measurements, to focus on the possible magnetic peaks. At 3 K, *q* scans along (100), (110) and (111) directions were conducted, during which the strong magnetic peaks at (111) and $(11\bar{1})$, and structural peak at (200) were detected. Note that, the (111) peak is also allowed structure peak of SCMO, however the intensity is roughly three-order smaller than the strongest peak. There might be some magnetic contribution to (200) peak, which is concealed by the strong substrate $SrTiO_3$ (100) peak. We further traced the magnetic (111), $(11\bar{1})$ and structure (220), (400) peaks during heating up to 500 K. A clear magnetic transition at ~ 120 K was observed, which is probably due to the strong Cr-Mo anti-site defects.

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Unconventional pairing states from fluctuating order: Role of superconducting fitness

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We study unconventional pairing mediated by nearly critical fluctuations of a non-superconducting order parameter that involves multiple degrees of freedom. This is motivated by the observation that superconductivity often appears close to other ordered states in experimental phase diagrams. We propose a general theory in the weak coupling regime that qualitatively connects the pairing strength with the compatibility of the pairing states and the fluctuating orders. The key ingredients are the time-reversal symmetry of the order and the superconducting fitness function. We prove our theory is universal for any electron-electron interaction which is sufficiently peaked in momentum space about the ordering vector. Our theory is applied to the spin-1/2 and spin-3/2 systems accounting for the fermiology. We propose that the superconducting fitness function can be used as a guide to identify unconventional pairing instabilities.