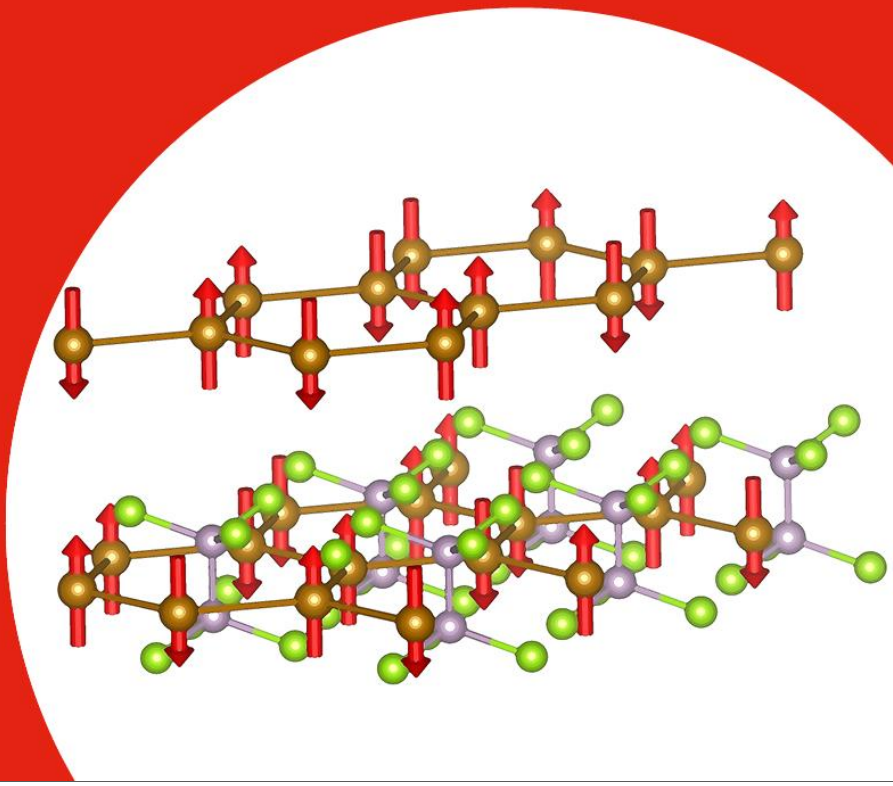
CRIM 2024:
Quantum Magnetism in Low-Dimensional Systems

27 September 2024
Institute of Physics, London, UK



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Exploring Entanglement and Putative Topological Order of Quantum Phases in Mixed-Range Interacting Quantum Spin Chains

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The quantum phase diagram of one-dimensional interacting spin chains gives rise to a wide zoo of complex phases. Here we investigate a quantum spin chain model with both short-range nearest-neighbour (NN) interactions and longer-range interactions, beyond next-NN. Frustration is enforced by the differing signs of the interactions and gives rise to non-trivial quantum phases within the system.

By engineering the novel interaction structure of the Hamiltonian, the transition point between the physics of trivial short-range interacting spin chains to complex long-range interaction regimes is studied. We explore the quantum phase diagram of this model using a density matrix renormalisation ground (DMRG) approach to utilise the matrix product state (MPS) representation of the ground state for this work. The entanglement structure within the MPS is probed with quantum information measures, in order to classify the quantum phases and identify the phase transition points.

The effectiveness of certain information-theoretic measures in finite-length chains is evaluated and signatures are detected that suggest topologically non-trivial phases. Those that are robust to symmetry-breaking perturbations, contain a high degree of entanglement across the chain, and which also possess protected degenerate ground states separated by a gap in the energy spectrum. We find that by introducing truncation within long-range interacting spin chain systems, we retain similar features of all-to-all connectivity, but display unique characteristics depending on the truncation range.

This work highlights the interplay between short-range and long-range interactions and the structure of quantum phases that arises. It can be used to offer further insight into the engineering of qubits for exploiting the non-local protection properties of topologically ordered phases of matter.

Magnetic properties of frustrated fcc oxides with general formula A2GdMO6 (A = Ba, Sr, Ca; M = Sb, Nb) for cryogenic refrigeration

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It is crucial to explore magnetic refrigeration as an alternative to vapour-compression refrigeration because the latter requires greenhouse gases, ozone depletors and/or gases from finite sources, such as helium. Nowadays, liquid He and 3-He are most commonly used to achieve cryogenic temperatures. Magnetically frustrated compounds are promising candidates for solid-state refrigeration because their magnetocaloric performances are enhanced due to the suppressed ordering temperatures, high magnetic moments, large ground state entropy, and minimal nearest-neighbour (nn) spin interactions. Gadolinium oxides with a double perovskite structure in frustrated fcc lattices remain a relatively new field of research and are less investigated than the garnet and pyrochlore lattice analogues. Here we aim to investigate the role of d0 and d10 ions on the lanthanide superexchange by comparing the performances of two families of fcc gadolinium oxides: A2GdNbO6 and A2GdSbO6 (A = {Ba, Sr, Ca}). Zero field cooled (ZFC) magnetic susceptibility measurements on A2GdNbO6 compounds show that there is no evidence of magnetic ordering down to 1.8 K, indicating minimal short-range correlations. The compounds adhere well to the predicted Curie-Weiss behaviour for free uncoupled spins, with small ferromagnetic (Ba2GdNbO6) and antiferromagnetic (Sr2GdNbO6 and Ca2GdNbO6) deviations. The experimental effective magnetic moments of all compounds are in good agreement with the theoretical value for Gd3+ ions. Ca2GdNbO6 is found to be site-disordered, and the tuneability of its disorder is investigated in order to minimise the degree of correlations. Neutron magnetic PDF on Ba2GdSbO6 allowed to identify the AFM and FM Gd-Gd interactions in the sample down to 3.1 K. Correlations are present up to ~17 Å (figure attached). This corresponds to a span of approximately two unit cells, meaning that long-range ordering is still suppressed at 3.1 K. The overall results suggest that fcc gadolinium oxides are ideal candidates for the design of next generation magnetocaloric materials.

Quantum magnetism in the anisotropic kagome Y-kapellasite Y3Cu9(OH)19Cl8

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Y3Cu9(OH)19Cl8 materializes an anisotropic kagome model with 3 different nearest neighbor interactions, yielding a rich phase diagram [1]. Besides two long range ordered phases, a large area in this phase diagram, coined "jammed spin liquid" phase, which encompasses the isotropic kagome model, opens up. Noticeably the large difference in the Y and Cu radii prevents inter-site mixing and the anisotropic kagome planes are free from magnetic defects. We present a detailed investigation of large, phase pure, single crystals of this compound by neutron scattering, and local μSR and NMR techniques [2]. At variance with polycrystalline samples, the study of single crystals gives evidence for subtle structural instabilities at 33 and 13 K and a bulk magnetic transition at 2.1 K, well below the antiferromagnetic 100K Weiss temperature. The structural instabilities are attributed to the localization of one interlayer proton, preserving the kagome planes. At 2.1 K the compound shows a magnetic transition to the coplanar (1/3,1/3) long-range order as predicted theoretically. However, our analysis of the spin-wave excitations yields magnetic interactions, which locate the compound closer to the phase boundary to the spin-liquid phase than expected from ab initio calculations. Enhanced quantum fluctuations at this boundary may be responsible for the reduced ordered moment of the Cu2+ and hint at a strong effect of external perturbations.

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[2] D. Chatterjee et al , Phys. Rev. B 107, 125156 (2023)

High-Order Coupled Cluster Method (CCM): Phase Diagrams of Kitaev-Heisenberg-Type Models at Zero Temperature.

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The Coupled Cluster Method (CCM) is a powerful and flexible method of quantum many-body theory. Here, high-order CCM computer code (https://www-e.uni-magdeburg.de/jschulen/ccm/) written by Dr. Damian JJ Farnell is used to study two lattice quantum spin models at zero temperature. Key to the success of the method has also been an efficient parallelisation of the CCM code, carried out by Dr. Joerg Schulenburg at Otto-von-Guericke University, Magdeburg, Germany, which allows a (spatially) localised approximation scheme to be carried out to high orders of approximation. Results for the ground-state energy and order parameter are presented for spin-S Kitaev-Heisenberg (KH) model on the honeycomb lattice (https://arxiv.org/abs/2405.1437) and initial calculations (only) are described for the related spin-half compass model on the square lattice. Accurate estimates for the phase boundaries were found via the CCM for the KH model (see figure), where intermediate spin liquid phases were observed between magnetically ordered phases (Néel and zigzag; ferromagnetic and stripy) for the spin-1/2, spin-one, and spin-3/2 systems. Furthermore, two unexpected narrow phases are observed: one sandwiched between the zigzag and ferromagnetic phases and the other between the Néel and the stripy phases for the spin-half KH model. Initial results are described briefly also for the ground-state energy (etc.) and phase diagram of the spin-half compass model. Recent successes of the application of high-order CCM have also been in very large part due to fruitful and ongoing collaborations between Prof. Raymond Bishop (University of Manchester), Dr. Damian JJ Farnell (Cardiff University) and Prof. Johannes Richter (Otto-von-Guericke University, Magdeburg, Germany) – and more recently now also Dr. Ioannis Rousochatzakis (University of Loughborough) and Dr. Marios Georgiou (University of Leeds).

You'd better shape up: exploring topological magnetic excitations with implanted muons

Lancaster T

One theme in the field of low-dimensional magnetism is the understanding of magnetic phenomena in reduced dimensions using notions from topology. Examples of such phenomena include topological objects such as walls, vortices, merons and skyrmions, which can potentially exist as excitations in the spin textures of a range of systems. In recent years, the experimental discovery of skyrmions in magnetic materials and of their self-organization into a skyrmion lattice, together with their potential for use as high density, low-energy sensors and magnetic storage, has made the investigation of such magnetic topological objects particularly important [1].

I will discuss recent measurements of skyrmion systems where we have used implanted muons as a probe of their magnetism. I will survey our work in this area, but will concentrate on the centrosymmetric skyrmion host Gd2PdSi3 [2], where we find that spin fluctuations in the skyrmion-lattice phase are highly anisotropic, implying that spin anisotropy plays a prominent role in stabilizing this state. We also observe anisotropic spin dynamics in the ground-state incommensurate magnetic phase of this material, indicating that it hosts a meron-like multi-q magnetic structure.

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A carbon-based two-dimensional Kondo spin lattice at metal-organic molecule interfaces

Ozdemir S

Fundamental studies on organic molecules have offered playground for magnetic order that is not limited to low temperatures1, with metal-molecule interfaces incorporated into thin film structures being the more promising direction for device integration2,3. Recent scanning tunnelling spectroscopy experiments have provided evidence for an ultra-high vacuum emergence of a molecular Kondo spin lattice at textured metal – organic molecule interfaces4–6. I will be showing evidence of emergence of two-dimensional Kondo spin lattice at epilayer Pt and Pt/Co – organic molecule interfaces away from a high-vacuum environment. A temperature dependent planar magnetisation onset due to molecular lattice of spins is observed, accompanied by magnetic frustration and anomalous Nernst effect in the vicinity of the phase transition7. Experimental data point towards a Kondo spin lattice in localised limit, where experimental signatures of the spin liquid state are expected to be manifested8.

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Structure and magnetism in the organometallic quantum magnet Cu-CPA

Philippe J[1,2], Elson F[3], Casati N[2], Sanz S[4], Metzelaars M[4,5], Shliakhtun O[1,2], Forslund O[1,6], Lass J[2,7], Shiroka T[2], Linden A[1], Mazzone D[2], Shin S[2], Medarde M[2], Lake B[9,10], Mansson M[3], Ollivier J[8], Bartkowiak M[2], Normand B[2,7], Kögerler P[5], Sassa Y[11], Janoschek M[1,2], Simutis G[2]
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Quantum spin ladders bridge the gap between one and two dimensions and have complex excitation spectra, which depend on the relative strengths of the leg and rung exchange interactions. While the realization of strong-rung ladders is fairly common, strong-leg ladders are a much rarer occurrence. In this contribution, we study an organometallic one-dimensional magnet (CPA)2CuBr4, (Cu-CPA) first reported in [1] and proposed to realize the strong-leg spin ladder model.

Through detailed bulk measurements and scattering experiments, we have discovered previously unknown structural phase transitions that take place below 200 K. The low-temperature structure that gives rise to the magnetic properties is described as a double spin ladder [2]. We will report the detailed structure of the ladder and discuss the implications of this structure on the magnetic properties. Finally, we will discuss our ongoing detailed investigations of the low-temperature magnetism.

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Kitaev materials in van-der-Waals heterostructures

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The booming interest in quantum technologies and neuromorphic computing is driving the search of exotic phases of matter for futuristic applications. The recent discovery of van der Waals (VdW) materials that approximate the intriguing physics of quantum spin liquids has attracted a large deal of interest. Simultaneously, the capability of controlling the twist angle between stacked VdW materials and producing moiré superlattices (MSLs) has opened the possibility of engineering quantum phases with no counterpart in Nature. Here we show that twisted bilayers of (Kitaev) quantum spin liquids, can exhibit unique phases as a function of the interlayer coupling. By constructing a mean-field approximation in terms of solutions of commensurate bilayers, we show that the band structure of deconfined spinons is greatly modified and exhibits nearly perfectly flat bands featuring a very large local (spinon) density of states that could potentially be probed in STM experiments. We also discuss the theory for 2D-to-2D tunneling spectroscopy by in graphene/monolayer $RuCl_3$ and signatures of quantum magnetic excitations.

Model of ultrafast excitation in 2D magnets: Generalized two- temperature model

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Since the discovery of magnetic ordering in two-dimensional systems, the family of two-dimensional van der Waals magnetic materials (2D vdW) has been considerably enriched, comprising now all types of magnetic ordering: ferromagnets, antiferromagnets and even ferrimagnets. Recently the interaction of 2D materials with ultrafast laser pulses has been more and more investigated both experimentally and theoretically Refs. [1-4].

We propose an improved model that is able to reproduce the type-II [5] ultrafast demagnetisation dynamics observed in 2D systems. The spin system is coupled to the electronic thermal bath and it is treated within the atomistic spin dynamics via the software package VAMPIRE[6], while the electron and phonon heat baths are described phenomenologically by coupled equations, also known as the two-temperature model.

Our proposed two-temperature model takes into account the effect of the heated substrate, which for 2D systems results in a slow demagnetisation regime. Since the substrate has different specific heats than the magnetic system, it will heat up more slowly and will lead to a slow demagnetisation of the

magnetic system. We applied the framework to a generic 2D system, CrI3, and we are able to observe a type-II demagnetisation process, characterised by two steps, the first step being attributed to the free electrons generated when the system behaves as a quasi-metal under optical excitation, and the second step, the slower demagnetisation region, due to the heated substrate. After laser excitation, we are able to observe domain formation, similarly to experimental observation[2]– inset Fig.1 – proving that also in the case of type-II dynamics domain formation is possible. Finally, we are able to study the domain formation and type-II ultrafast magnetisation dynamics for various fluences and values of the spin damping as shown in Fig. 1.

Magnetic Properties of Non-Linear Spin-1 Chains with Staggered and Chiral Single-Ion Anisotropy Directions

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Spin-1/2 staggered AFM chains, in which the orientation of the local spin environment alternate site to site, are known to exhibit magnetic properties which differ greatly from their linear counterparts. The non-trivial staggered g-tensor and the Dzyalonshinskii-Moriya (DM) interaction present in these systems, give rise to a field-induced spin-gap and a rich low-temperature excitation spectrum containing breather and soliton modes [1,2,3], which were accounted for by mapping the Hamiltonian to the sine-Gordon quantum-field theory [4,5]. More recently, experiments on a chiral spin-1/2 AFM system, with a four-fold chiral modulation of the local spin environment, found a similarly rich excitation spectrum and field-induced spin-gap which departs from the predictions of the sine-Gordon model and remains to be fully explained [6].

Despite such unique phenomena displayed by non-linear spin-1/2 chains, investigations into the effects of an alternating spin environment on AFM spin-1 chains, which adopt complex ground states that differ fundamentally [7], are notably lacking. In addition to the aforementioned staggered g-tensors and DM interaction, these spin-1 systems are expected to host a single-ion-anisotropy direction which also vary site to site and act in competition with the exchange interactions. Here we present the results of magnetometry, neutron diffraction and inelastic neutron scattering data on spin-1 staggered and chiral systems, Ni(pyrimidine)(NO3)2(H2O)2 and [Ni(pyrimidine)(H2O)4]SO4 respectively.

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The magnetic Hamiltonians for the layered transition metal-PS antiferromagnets: successes and failures

Wildes A

The TM-PS (TM = Mn, Fe, Co, Ni) family of compounds are layered van der Waals magnets. They have been extensively studied in the past but are now the subject of renewed interest as they are intrinsically magnetic and, like graphite, can be delaminated down to monolayer thicknesses. The compounds are isostructural, with the transition metals forming a honeycomb lattice in the quasi-two-dimensional planes, but they show remarkably different magnetic behaviour. Ordered magnetic structures, magnetic anisotropies and exchange constants, and magnetic critical properties vary considerably with the transition metal, essentially a result of removing electrons one at a time from a half-filled d shell. The differences could be
understood if appropriate magnetic Hamiltonians could be determined. Knowledge of representative Hamiltonians is also essential information for the suitability of these compounds in device applications. Experiments to test the magnetic Hamiltonians for the TM-PS compounds will be summarised, with particular emphasis on neutron inelastic scattering, and an opinion on the outstanding problems to be solved in determining appropriate Hamiltonians will be expressed.

Mapping of the non-equilibrium behavior of the Anderson impurity model to an effective model using machine learning

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Magnetic Tunnel Junctions (MTJs) are layered heterostructures of strongly-correlated materials that behave like artificial neurons under a voltage switch, and are used as functional components in neuromorphic hardware. To design better MTJs, and thereby better neuromorphic networks built from them, we would like to be able to simulate the nonequilibrium switching process, starting from a microscopic model of candidate devices. This is a challenge since one has to account for strong electron interactions, magnetism, and interfacial effects in the setting of a quantum quench. Dynamical mean field theory (DMFT) provides a route to such simulations, and the Anderson Impurity Model (AIM) is the underlying model. Here we investigate quench dynamics in the AIM relevant to electrical actuation of the MTJ, using an effective representation first introduced in [1], in an equilibrium setting. By combining a range of techniques (ED, DMRG, NRG) on the interacting system, we use machine learning methods to obtain an efficient noninteracting representation, and study its properties. Our findings may help understand the microscopic processes of quenches and hence facilitate MTJ design.

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Pressure-induced Structural, Magnetic and Electrical Evolution in the Triple-Layer Stacked van der Waals Antiferromagnet FePSe3

Deng S

Layered van der Waals compounds have been increasingly popular in recent decades. One particular class, magnetic van der Waals compounds, provide the ideal platform to study strongly correlated electrons in low dimensions. FePSe3 has been reported to undergo insulator-to-metal and superconducting transitions with the application of pressure recently. We comprehensively investigated the pressure-induced evolution of crystalline, magnetic structures and the transport properties using different experimental probes. Our work provides an unambiguous structural transition model for
FePSe3 under pressure from R-3 to R3, losing the inversion center, concomitant with the emergent metallicity and thus might potentially inducing polar metallicity. The HP phase at low temperatures is excluded from any magnetic ordering in our neutron diffraction data. We consolidate our results into a comprehensive temperature-pressure phase diagram of FePSe3.
Deng S 1,2 , Coak M 3 , Haines C 4 , Hamidov H 1,5 , Jarvis D 1,2 , Zhang X 1 , Liu C 1 , Daisenberger D 6 , Warren M 6 , Hansen T 6 , Klotz S 7 , Kim C 8 , Yang P 9, 10 , Wang B 9, 10 , Guang J 9, 10 , Park J 8 , Wildes A 2 , Saxena S 1, 11
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S = 1⁄2 Kagome Magnets in the Two-Dimensional Limit

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2017 saw the publication of two landmark studies demonstrating the detection of intrinsic ferromagnetism in two-dimensional (2D) layers of CrI_3 and $Cr_2Ge_2Te_6$.[1,2] Since then, there has been growing interest in 2D magnetic materials, whose low dimensionality gives them the potential to host exotic magnetic behaviour and topological states of matter.[3] Magnetic metal-organic nanosheets (MONs) are a class of two-dimensional materials which are highly tuneable[4] and obviate magnetic site disorder; an issue purely inorganic systems often suffer from.[5] In this poster we highlight MOF-bipy ($Cu_3(CO_3)_2(C_{10}H_8N_2)_6 \cdot 2ClO_4$), a layered metal-organic framework (MOF) with S = 1/2 Cu2+-containing kagome layers connected to monodentate ligands in the crystallographic c-direction, where these layers are held together by weak intermolecular forces. Here we elucidate its magnetic structure as ferromagnetic kagome layers which are ferromagnetically correlated to adjacent layers. We also demonstrate that the weak intermolecular forces between layers can be overcome using Scotch tape exfoliation, yielding few-layer MONs with lateral dimensions on the order of hundreds of nanometres. These MONs host the potential to be characterised at the 2D limit using techniques such as X-ray magnetic circular dichroism (XMCD).

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Spin dynamics in the magnetically ordered state of the RbNiCl3 Haldane chain

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Research in one-dimensional antiferromagnets with low-spin number gained significant interest following Haldane's conjecture [1] and the subsequent 2016 Nobel Prize in Physics. This work focuses on RbNiCl3, a hexagonal lattice crystal with nickel ions forming antiferromagnetic chains along c-direction, it is a highly one-dimensional system where long-range order is not possible due to strong quantum fluctuations.

To study the dynamics of these systems, inelastic neutron scattering is the most effective method. While previous studies on RbNiCl3 have been conducted [2], the latest advancements in this technique, particularly with the multiplexing spectrometer (CAMEA) at the SINQ neutron source, offer an opportunity for a deeper understanding of the system.

The goal of this research is to build the most reliable model possible by comparing experimental and simulated data and determining all the magnetic interactions and their corresponding strengths.

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Understanding synthesis-driven structure-magnetic property relationships in zinc vanadate

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Quantum materials are strongly correlated electron systems with lattice, charge, spin and orbital degrees of freedom giving rise to novel states of matter that have a non-trivial quantum mechanical origin. Exotic states can arise in quantum magnets where $S \leq 1$ spin centres are connected in low-dimensional and/or geometrically frustrated systems. For example, quantum spin liquids (QSL) have been observed in the geometrical frustrated pyrochlore lattice of cubic spinel zinc vanadate, ZnV_2O_4. This compound has strong magnetic frustration and orbital degeneracy in the V^{3+} ion, which leads to complex behaviour. This includes a cubic to tetragonal phase transition at TS, up to two magnetic phase transitions at T1 and T2 and unknown disordered magnetic ground states.1-6 The temperatures of these transitions, and whether or not they take place, depends on the synthesis method for reasons that remain uncertain. In this work, we investigate synthesis dependent microstrain as the cause of these variations in properties.

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Structure and magnetism in the organometallic quantum magnet Cu-CPA

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Quantum spin ladders bridge the gap between one and two dimensions and have complex excitation spectra, which depend on the relative strengths of the leg and rung exchange interactions. While the realization of strong-rung ladders is fairly common, strong-leg ladders are a much rarer occurrence. In this contribution, we study an organometallic one-dimensional magnet (CPA)2CuBr4, (Cu-CPA) first reported in [1] and proposed to realize the strong-leg spin ladder model.

Through detailed bulk measurements and scattering experiments, we have discovered previously unknown structural phase transitions that take place below 200 K. The low-temperature structure that gives rise to the magnetic properties is described as a double spin ladder [2]. We will report the detailed structure of the ladder and discuss the implications of this structure on the magnetic properties. Finally, we will discuss our ongoing detailed investigations of the low-temperature magnetism.

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