A quantum spin–liquid phase is an intriguing possibility for a system of strongly interacting magnetic units in which the usual magnetically ordered ground state is avoided owing to strong quantum fluctuations. It was first predicted theoretically for a triangular–lattice model with antiferromagnetically coupled $S=1/2$ spins. Recently, materials have become available showing persuasive experimental evidence for such a state. Although many studies show that the ideal triangular lattice of $S=1/2$ Heisenberg spins actually orders magnetically into a three–sublattice, noncollinear 120 arrangement, quantum fluctuations significantly reduce the size of the ordered moment. This residual ordering can be completely suppressed when higher–order ring–exchange magnetic interactions are significant, as found in nearly metallic Mott insulators. The layered molecular system kappa–(BEDT–TTF)$_2$Cu$_2$(CN)$_3$ is a Mott insulator with an almost isotropic, triangular magnetic lattice of spin–$1/2$ BEDT–TTF dimers that provides a prime example of a spin liquid formed in this way. Despite a high–temperature exchange coupling $J = 250$ K, no obvious signature of conventional magnetic ordering is seen down to 20 mK. Here we show, using muon spin rotation, that applying a small magnetic field to this system produces a quantum phase transition between the spin–liquid phase and an antiferromagnetic phase with a strongly suppressed moment. This can be described as Bose–Einstein condensation of spin excitations with an extremely small spin gap. At higher fields, a second transition is found that suggests a threshold for deconfinement of the spin excitations. Our studies reveal the low–temperature magnetic phase diagram and enable us to measure characteristic critical properties. We compare our results closely with current theoretical models, and this gives some further insight into the nature of the spin–liquid phase.
Probing quantum magnetism using coordination polymers and pulsed magnetic fields

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Although much current technology is based on rather simple inorganic compounds, there is growing interest in employing organic and molecular groups to assemble arrays of coupled transition metal ions, principally copper, nickel and cobalt, into novel architectures. In these metal–organic coordination polymers, the transition metal ions are used to provide the magnetic moment, but organic groups mediate the interactions. This allows the development of extremely well-controlled materials in which the dimensionality, coupling strength and lattice geometry can be adjusted and facilitates the testing of new theoretical models of quantum magnetism. High magnetic field measurements of these materials show that their properties are very strongly dependent on details of their structure. Magnetization in pulsed magnetic fields up to 60T is used to study the dimensionality of these systems and extract interaction energies.
The RFe2O4 compounds exhibit simultaneously charge ordering (CO) of the Fe2+ and Fe3+ ions [1], together with magnetic ordering of the Fe spins [2] and possible multiferroic behaviour [3]. Synchrotron data collected below the 3D CO transition show intensity concentrated around peaks separated by ~1/3 c* but slightly displaced in the (a*, b*) plane. Calculations modelling an oxygen displacement pattern are in excellent agreement with the data, suggesting an incommensurate CO of the Fe ions close to the commensurate sqrt (3) X sqrt(3) structure and associated with a helical strain pattern. At high temperature, degenerate propagation vectors corresponding to many different displacement patterns are simultaneously populated by the system leading to helices of scattering in reciprocal space.

Polarized neutron scattering is a powerful technique that can unveil details of complex magnetic structures not accessible through conventional scattering techniques. New details about Ni$_3$V$_2$O$_8$ (NVO) magnetic structures are revealed using unpolarized and polarized neutron diffraction data. By complementing polarized neutrons with electric polarization measurements, we demonstrate direct electric control of multiferroic domains in NVO. A comprehensive qualitative and quantitative analysis indicates that magnetic and ferroelectric domains coincide at low temperatures and can be controlled by an external electric field, a desired feature in the design of future spin logic devices. Finally, I will present evidence for an unusual `memory effect' in NVO's multiferroic phase, where a previously electrically-polarized sample reestablishes its polarization direction upon exiting and re-entering the multiferroic phase in the absence of a field.
The momentum–resolved magnetic spectrum of many hole–doped copper oxides, including both superconductors and non–superconductors, exhibits a characteristic hour–glass shape. The origin of this feature has been debated for over a decade. We have recently observed the same hour–glass spectrum in neutron scattering measurements of the hole–doped antiferromagnet La2–xSrxCuO4, which has stripe correlations and is an insulator [A. T. Boothroyd et al., Nature 471, 341 (2011)]. The hour–glass spectrum of La2–xSrxCuO4 bears a remarkable similarity with that of the hole–doped superconductors. The results provide strong evidence that slowly fluctuating stripes cause the hour–glass spectrum in the copper oxide superconductors.
Direct observation of charge order in triangular metallic AgNiO2 by single-crystal

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We report resonant x-ray scattering measurements on a single crystal of the orbitally degenerate triangular metallic antiferromagnet 2H–AgNiO2 to probe the spontaneous transition to a triple-cell superstructure at temperatures below $T_S = 365$ K. We observe a strong resonant enhancement of the supercell reflections through the Ni K edge. The empirically extracted K-edge shift between the crystallographically distinct Ni sites of $2.5(3)$ eV is much larger than the value expected from the shift in final states, and implies a core-level shift of $1$ eV, thus providing direct evidence for the onset of spontaneous honeycomb charge order in the triangular Ni layers. We also provide band-structure calculations that explain quantitatively the observed edge shifts in terms of changes in the Ni electronic energy levels due to charge order and hybridization with the surrounding oxygens.
We study quantum phase transitions in 2D systems in which the "topological order" of the zero-temperature quantum many-body wave function changes. We discuss the critical theory, and identify model Hamiltonians in which such transitions arise. This talk will focus on one such example which can be realized in a bilayer chiral $p$-wave superconducting system.
Advances in compound prediction methodology have made it possible to identify new synthesizable compounds with little or no input from experiment. Using a combination of ab initio high-throughput and evolutionary searches [1] we have found new candidate ground states at 1:4 and 1:2 compositions in the well-known Fe–B system. The uniqueness of the proposed crystal structures gives rise to a set of remarkable properties: oP12–FeB$_2$ is expected to be the first semiconducting metal diboride and oP10–FeB$_4$ is shown to have the potential for phonon-mediated superconductivity with a T$_c$ of 15–20 K [2]. In addition to exhibiting unusual electronic features, the two compounds might be harder than the known Fe–B materials commonly used for hard coating applications. Finally, we examine synthesis routes that could be used to discover the proposed crystal structure phases [3].

Quantum information processing offers one of the most exciting challenges in the study and development of nanomaterials. It is at the cutting edge of quantum nanoelectronics, and we are part of the world wide race to develop a scalable quantum computer. We need materials with quantum states that can be individually controlled and measured, and yet which are sufficiently robust against decoherence that they can sustain a sequence of quantum manipulations and interactions. We lead the world in using the new family of fullerene materials (popularly known as Bucky balls), which can be used to contain atomic and molecular species inside a cage that separates them from the quantum environment. We can insert fullerenes into carbon nanotubes to create one-dimensional 'peapod' arrays, which we can image by aberration corrected high resolution transmission electron microscopy, and we are also developing other schemes for molecular self-assembly of fullerenes and other functional molecules. We can also use other materials such as doped silicon and diamond. We can store the quantum information in electron or nuclear spin, and exchange it between the two. We can manipulate and characterize the spin states by electron paramagnetic resonance and also optically. By creating entanglement between several spins, it will be possible to develop sensors that exceed the standard quantum limit. By storing information holographically in collective spin states, it will be possible to process quantum information in large ensembles of spins.
Interplay of superconducting, magnetic and structural order parameters in NaFe$_{1-x}$Co$_x$As

Jack Wright
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The recently discovered Fe-based superconductors have attracted a great deal of experimental and theoretical interest and now rival the cuprates as striking examples of unconventional superconductivity. One of the most important features of these materials is the ability to tune a magnetic parent compound into a superconducting state via chemical doping and the competition and/or coexistence of magnetic and superconducting phases is one of the field’s most hotly debated topics. Here we present the results of a detailed study of the pnictide system NaFe$_{1-x}$Co$_x$As. We observe how the emergence of a superconducting state, on increasing $x$, affects magnetic and structural order parameters, and vice-versa, as revealed by synchrotron x-ray diffraction and muon spin rotation (muSR).
Magnetic resonances in Fe(Se,Te) superconductors

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A common feature in many high–Tc superconductors is the emergence of a sharply peaked mode below Tc localised in momentum and energy space. The precise origin of this mode is still a subject of debate but the existence of a superconductivity–induced spin resonance has been shown to relate to the superconducting state and gap symmetry. In our work we have used inelastic neutron scattering to probe the magnetic spin dynamics of optimally doped sample of FeSe0.5Te0.5 and magnetic but non–superconducting Fe1.1Se0.25Te0.75. By this method, we demonstrate that the resonance is intimately connected to the superconducting state and using polarised neutrons ascertained the symmetry of the gap function.
Local microstructural variations in thin film and single-crystal FeySe$_{1-x}$Tex

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Oxford Materials

Chemical composition and strain are known to greatly affect the superconducting and magnetic properties of Fe(Se,Te) compounds. However, in most cases, only average composition values and structural parameters based on bulk analysis are available. In the Materials Department we have been investigating local microstructural variations in both thin films grown in-house and single crystals grown elsewhere (Bendele et al., 2010) in an attempt to improve understanding of the relationships between chemical composition, strain and properties. Local changes in composition have been studied using extensive EDX microanalysis in a Scanning Electron Microscope, and a sophisticated high-resolution Electron Backscatter Diffraction (HR-EBSD) technique has been used to evaluate changes in strain over micron-scale distances. These studies show that there are significant chemical and structural changes on a fine-scale within “single crystal” samples.

The role of the dopant on the magnetic phase diagram of LaO(1−x)FxFeAs

Harry Fisher
Oxford Materials

Within the framework of ab initio density functional theory calculations, we investigate how the magnetic ground state of LaO(1−x)FxFeAs evolves as a function of F content. Simple models of the doping, such as the rigid band approximation, fail to accurately describe the relationship between fluorine content and magnetic order. Here we show that by using a large supercell where fluorine atoms are explicitly included, it is possible to reproduce a magnetic–nonmagnetic transition in qualitative agreement with experimental observations.

We also examine the atomistic origin of the magnetic–nonmagnetic transition, and clarify the roles of the Fe–As distance and the additional electronic charge in the magnetic phase diagram of LaO(1−x)FxFeAs.
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