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Abstracts

Talks

Assembling, Understanding And Auguring Phase Diagrams for Fe-Based Superconductivity

Paul Canfield
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The quest for improved examples of novel, potentially useful, superconductors reached another milestone in 2008 with the discovery of Fe-based superconductivity in wide range of structurally related arsenide and selenide compounds. In particular, the AFe$_{2}$As$_{2}$ (A = Ba, Sr, Ca) compounds proved to have the highly desirable combination of intriguing properties that imply intimate coupling between electronic, magnetic and structural degrees of freedom, exceptionally high and relatively isotropic upper critical field curves and readily grown, homogeneous single crystals. Over the past three years the CMP community has been able to develop a broad and deep empirical understanding of substitutional and pressure based phase diagrams of these materials that is leading to theoretical as well as synthetic insights. In this talk I will broadly review some of our key findings and speculate about future directions for research in this field.

Magnetism, Superconductivity and Chemistry of Layered Non-Oxide Solids

Simon Clarke
Oxford Chemistry

A series of layared manganite oxide chalcogenides will be described which present competing magnetic ground states and structural order and which have compositions which can be oxidised or reduced in a continuous way in order to tune the physical properties by changing the ratio of Mn2+ and Mn3+ oxidation states. These materials provide a counterpoint to the better studied Mn3+/Mn4+ oxides which show complex magnetism. The use of chemical methods to tune the properties of iron-based superconductors will also be described.

Crystal Growth at Oxford Physics Using Floating Zone

Prabhakaran Dharmalingam
Oxford Physics

Recent discoveries of new materials with exciting properties such as Fe-based superconductors, multiferroics, spin ice and topological insulators have increased the interest and demand for crystals these days. In order to accommodate this demand, we here at the Clarendon Laboratory, have expanded our crystal growth facilities.

In addition to the existing instruments, we now also have a new optical floating-zone light furnace, 40KW MF Czochralski puller, and a three zone furnace. In this talk, I will briefly explain about our recent work.

Low-Temperature Topochemical Reduction as a Route to Novel Electronic Materials

Michael Hayward
Oxford Chemistry

Complex transition metal oxides have been of longstanding interest due to the wide range of physical properties they exhibit. Much of the complex behavior observed in these phases arises from strong coupling between the electronic states on neighboring metal centers. This coupling is generally mediated and facilitated by the orbitals of the intervening oxide anions and is therefore strongly influenced by the topology and geometry of the transition metal-oxygen network.

In the search for new electronic materials and phenomena, one fruitful approach is to prepare phases with novel metal-oxygen networks. Unfortunately the high-temperature synthetic techniques conventionally utilized in the preparation of complex transition metal oxides tend to be restricted to the preparation of thermodynamic phases. These phases tend to exhibit only a limited repertoire of metal oxidation states, coordination geometries and three dimensional packings and as a result high-temperature syntheses can only realize a small fraction of the metal-oxygen frameworks (and thus electronic materials) which may be considered 'stable'.

Low-temperature topotactic reduction reactions utilizing binary metal hydrides as reducing agents allow the anion lattices of complex transition metal oxides to be manipulated, while the topology of the cation lattice remains largely unchanged. The resulting metastable phases can exhibit highly unusual transition metal oxidation states and coordination geometries and contain metal-oxygen frameworks which cannot be prepared by high-temperature routes.

We have recently exploited this synthetic approach to prepare a series of phases containing transition metal centers in unusual coordination geometries and oxidation states, which give rise to novel configurations of the localized d-electrons present in these materials.

Thin Film Growth Using Molecular Beam Epitaxy

Thorsten Hesjedal
Oxford Physics

I will present an update on the advanced materials growth facilities at the Research Complex at Harwell (RCaH). Single-crystal films and nanostructures can be grown by molecular beam epitaxy (MBE), UHV sputtering, and chemical vapour deposition (CVD). Our focus is currently on epitaxial selenide, telluride, and oxide thin films.

Quantum Ice

Nic Shannon
Oxford Physics

"The "spin ice" state found in the rare earth pyrochlore magnets Ho2Ti2O7 and Dy2Ti2O7 offers a beautiful realisation of classical magnetostatics, complete with magnetic monopole excitations.
We have recently used quantum Monte Carlo simulation to demonstrate how tunnelling between different ice configurations stabilizes a quantum spin liquid state in which this classical magnetostatics gives way to fully-fledged electromagnetism, complete with magnetic "photon" excitations [1].

Here we take a more practical second look at the problem, exploring how such state might manifest itself in a qunatum spin ice material [2].

[1] Nic Shannon et al., Phys. Rev. Lett. 108, 067204 (2012)

[2] Owen Benton et al., in preparation.

Spin Waves and Revised Crystal Structure of Honeycomb Iridate Na2IrO3

Sungkyun Choi
Oxford Physics

We report inelastic neutron scattering measurements on Na2IrO3, a candidate for the Kitaev spin model on the honeycomb lattice [1]. We observe spin-wave excitations below 5 meV with a dispersion that can be accounted for by including substantial further-neighbor exchanges that stabilize zigzag magnetic order. The onset of long-range magnetic order below TN=15.3 K is confirmed via the observation of oscillations in zero-field muon-spin rotation experiments. Combining single-crystal diffraction and density functional calculations we propose a revised crystal structure model with significant departures from the ideal 90° Ir-O-Ir bonds required for dominant Kitaev exchange [2].

[1] J. Chaloupka, G. Jackeli, and G. Khaliullin, Phys. Rev. Lett. 105, 027204 (2010).

[2] S. K. Choi, R. Coldea, A. N. Kolmogorov, T. Lancaster, I. I. Mazin, S. J. Blundell, P. G. Radaelli, Yogesh Singh, P. Gegenwart, K. R. Choi, S.-W. Cheong, P. J. Baker, C. Stock, and J. Taylor, Phys. Rev. Lett. 108, 127204 (2012)

Controlling Magnetic Dimensionality with Applied Pressure

Saman Ghannadzadeh
Oxford Physics

Metal-organic coordination polymers are self-assembly materials in which transition metal ions are linked via organic molecules into chain or plane-like structures. Strong hydrogen bonds enable these units to form three-dimensional lattices, while the underlying anisotropy causes low-dimensional magnetism to evolve. Through coordination chemistry we have begun to gain chemical control over these systems, allowing us to modify the exchange ligands or the transition ions, while still maintaining the same basic magnetic network. This gives a good degree of control over properties such as the magnetic anisotropy [1], making these materials ideal candidates for use in purpose-engineered magnetic systems. Furthermore, exploring the relationship between the structure, physical and magnetic properties of these systems allows us to gain an understanding of the nature of the exchange interactions and the electronic correlations that give rise to the low-dimensional magnetically ordered phases of matter.

One material which we have focused on is CuF2(H2O)2(pyz)2 (pyz=pyrazine) [2]. This is a Cu-II co-ordination polymer, in which strong hydrogen bonds exist between the copper pyrazine chains, leading to two-dimensional magnetic properties at ambient pressure. This system has an active Jahn-Taller centre, where the magnetic orbitals are elongated along a particular axis, allowing the magnetic properties to be selectively modified through perturbation of the co-ordination environment. We have recently carried out high pressure measurements up to 20 kbar at the National High Magnetic Field Laboratory, using a modified radio-frequency technique which can be used to extract the absolute magnetisation [3]. Recent structural and low-field susceptibility measurements have suggested that CuF2(H2O)2(pyz)2 undergoes a phase transition with the application of pressure [4]. We will show that pressure can be used to switch the Jahn-Teller axis, and hence modify the orbital orientation and the magnetic properties; leading to a sharp transition from two-dimensional to one-dimensional magnetism at 9.1 kbar.

[1] P. A. Goddard, J. L. Manson, J. Singleton, I. Franke, T. Lancaster, A. J. Steele, S. J.

Blundell, C. Baines, F. L. Pratt, R. D. McDonald, et al., Phys. Rev. Lett. 108, 077208 (2012

[2] J. L. Manson, M. M. Conner, J. A. Schlueter, A. C. McConnell, H. I. Southerland, I. Malfant, T. Lancaster, S. J. Blundell, M. L. Brooks, F. L. Pratt, et al., Chemistry of Materials 20, 7408 (2008)

[3] S. Ghannadzadeh, M. Coak, I. Franke, P. A. Goddard, J. Singleton, and J. L. Manson, Review of Scientific Instruments 82, 113902 (pages 8) (2011)

[4] G. J. Halder, K. W. Chapman, J. A. Schlueter, and J. L. Manson, Angewandte Chemie International Edition 50, 419 (2011)

Half-Metallicity in the Ferrimagnet Nb(TCNE)2 from First Principles

Barbara Montanari
Rutherford Appleton Laboratory

Hybrid density-functional calculations performed on the metal-organic compound Nb(TCNE)2 (TCNE=tetracyanoethylene) confirm it to be a ferrimagnet with a high ordering temperature for a material of its class. Most interestingly, inspection of the electronic band structure reveals that the material is a half-metal. The structure investigated is formed by layers of Nb2+ ions and TCNE molecules, which are bridged by additional TCNE ligands. A delicate balance between strong on-site electron correlation characteristic of the electronic d states in Nb2+ and off-site hybridization with the TCNE molecules in the layers produces a half-metallic state. These spin-polarized Nb2+-[TCNE]·− layers are then coupled ferrimagnetically with the TCNE ligands above and below. The coexistence of intrinsic high-temperature ferrimagnetism and half-metallicity in a metal-organic compound is very relevant for the emerging area of half-metallic and organic spintronics.

Quantum Information Processing Using Electron Spins in Condensed Matter

Arzhang Ardavan
Oxford Physics

The quantum spins associated with electrons and nuclei, with their discrete quantum levels and weak interactions with other degrees of freedom, offer a natural class of systems for embodying quantum information. Many possible condensed matter electron-spin-based qubits have been examined, including, for example, paramagnetic defects and bound donors in semiconductors, self-assembled and lithographically defined quantum dots, and various paramagnetic molecular systems.

High spin systems (for which $S > 1/2$) with anisotropy, such as artificial molecular nanomagnets, offer the possibility of higher density information storage and may host quantum algorithms locally. We have studied the phase coherence of spin states in nanomagnets and optimised the phase memory time by chemical engineering of the molecular structures.

Traditionally, quantum spin states are manipulated using static and resonant magnetic fields. However, electrically-controllable spin qubits would offer substantial architectural advantages for the design of a quantum information processor because electric fields may be applied over shorter length scales than magnetic fields. Certain electron spins in condensed matter, for example those in molecular magnets exhibiting spin frustration, or those in environments with broken inversion symmetry, may be suitable candidates.

Real Time Read-out of Metastable States in a Superconducting Flux

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Royal Holloway, University of London

We report on real time measurements of macroscopic quantum states in superconducting flux qubits using a highly sensitive hybrid quantum interferometer as the readout probe. The readout device is a modified Andreev interferometer [1] with semi-metallic normal segment in a ``folded'' geometry, and is designed to reduce the back action during measurement, as well as minimising the electromagnetic coupling between the circuit and the environment.

A pulsed lock-in technique has been developed to perform continuous readout of the superconductor phase difference using pulse lengths down to 10 ns. The technique enables to control the energy of the probing quasiparticles in the normal segment of the interferometer, which in turn allows to control of the supercurrent flowing in the SNS loop and prevents electron heating of the normal segment.

The measurements show that two macroscopically distinct metastable states exist when the device is biased at the qubit degeneracy point, between which the system makes transitions that can be continuously monitored. Real time kinetics of the system has been investigated at different magnetic fluxes, pulse parameters, temperature and RF radiation. Based on statistical analysis of the transitions, we argue that the metastability is connected with macroscopic quantum tunnelling effects.

1. V. T. Petrashov, K. G. Chua, K. M. Marshall, R. Sh. Shaikhaidarov and J. T. Nicholls, Phys. Rev. Lett. 95 147001 (2005).

Time-Resolved Optical Pump-Probe Spectroscopy of Undoped and Dy-Doped BiFeO3 Multiferroic Thin Films

Katie Doig
Oxford Physics

Magnetoelectric multiferroics, with coupled electric and magnetic order parameters, have been of fundamental interest in recent years, with potential applications in information storage, spintronics and photovoltaics. BiFeO3 is widely studied as a room temperature multiferroic, in particular in thin film form, where compressive strain stabilises a tetragonal phase with higher saturation polarisation and magnetisation than in the bulk rhombohedral phase. Further improvement to the magnetisation has been achieved by substituting bismuth for lanthanides, modifying the incommensurate spiral spin structure; Dy doping has been particularly successful because of its relatively high magnetic moment.

We investigated the static and ultrafast optical properties of BiFeO3 thin films, which were grown by pulsed laser deposition on LaAlO3 (001) substrates. Pump-probe reflectivity spectroscopy (400nm pump, 800nm probe) monitored the ultrafast transfer of electrons from oxygen 2p to iron 3d states. The time-resolved reflectivity exhibited a fast (1ps) and a slow (>10ps) component, indicating the electronic relaxation time. Oscillations in the reflectivity were attributed to the propagation of a strain pulse through the film, created by electron-phonon coupling. The speed of sound in the doped and undoped samples was extracted from the oscillation frequency. Optical ellipsometry provided the refractive index and absorption coefficient, and gave insight into the electric-dipole active charge transfer transitions, which Dy-doping alters. In conjunction these techniques can be used to gain a better understanding of both the electronic properties and strain in multiferroic thin films, thereby enhancing their potential for applications.
of topical frustrated systems.

Homochiral Domains in BiFeO3

Roger Johnson
Oxford Physics

Through hard x-ray magnetic scattering, magnetic domains of up to several hundreds microns in size have been imaged at the surface of a ferroelectric mono-domain BiFeO3 single crystal; the most studied multiferroic to date. The domains correspond to cycloidal modulations of the magnetisation along the wave-vector $k=2\pi(\delta,\delta,0)$ and symmetry equivalent directions. The rotation direction of the magnetisation in all magnetic domains has been determined and found to be unique and in agreement with predictions of density-functional simulations. Furthermore, imaging of the surface shows that the largest adjacent domains display a 120 degree vortex structure.

Conventional Supercoductivity in SrPd2Ge2

Timur Kim
Diamond Light Source

Electronic structure of SrPd2Ge2 single crystals is studied by angle-resolved photoemission spectroscopy (ARPES), scanning tunneling spectroscopy (STS) and band-structure calculations within the local-density approximation (LDA). The STS measurements show single s-wave superconducting energy gap Delta(0) = 0.5 meV. Photon-energy dependence of the observed Fermi surface reveals a strongly three-dimensional character of the corresponding electronic bands. By comparing the experimentally measured and calculated Fermi velocities a renormalization factor of 0.95 is obtained, which is much smaller than typical values reported in Fe-based superconductors. We ascribe such an unusually low band renormalization to the different orbital character of the conduction electrons and using ARPES and STS data argue that SrPd2Ge2 is likely to be a conventional superconductor, which makes it clearly distinct from isostructural iron pnictide superconductors of the "122" family.