

# Solid State Group Christmas Meeting 2010

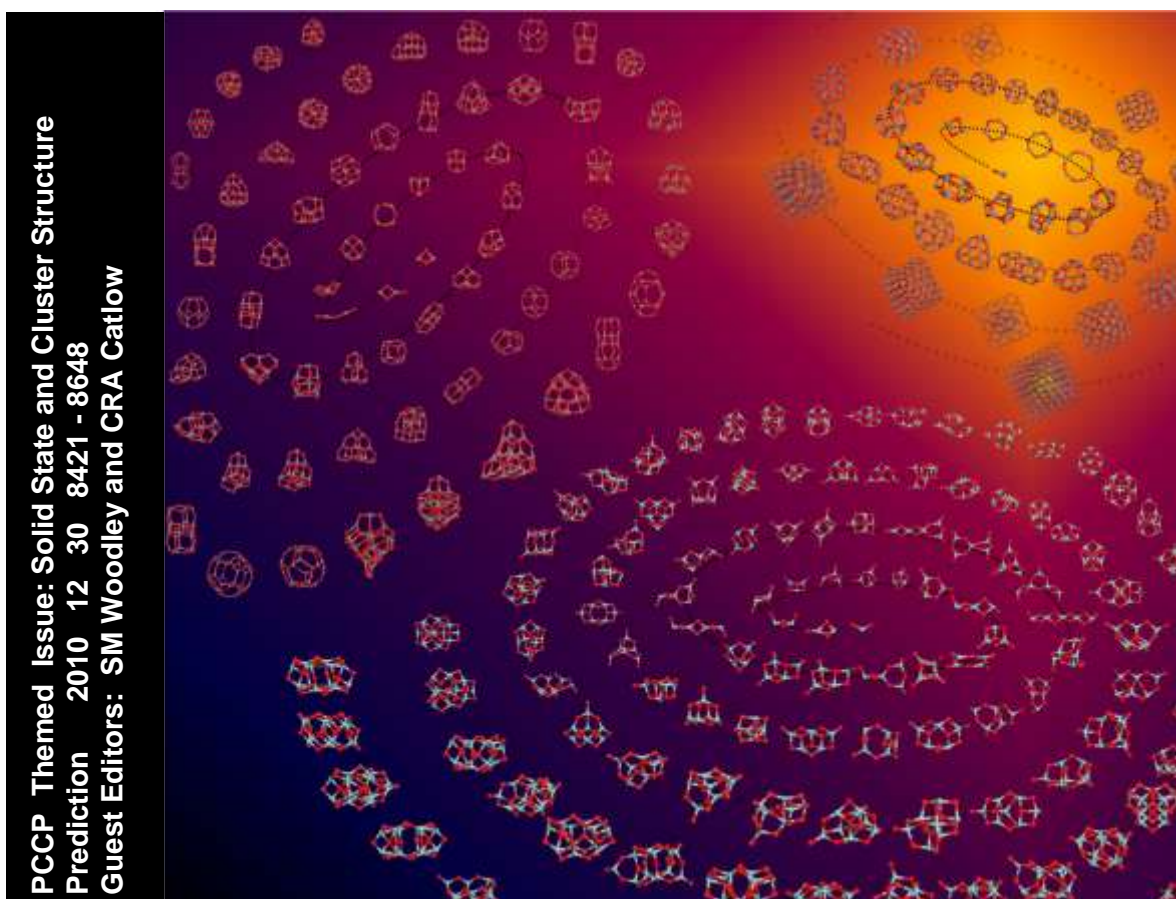
30<sup>th</sup> Anniversary of the First Polar Solids Discussion Meeting, 1980

UCL

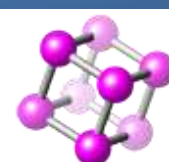
20<sup>th</sup>-21<sup>st</sup> December

Department of Chemistry, UCL, 20 Gordon Street, WC1H 0AJ

Scientific Talks:	Chemistry Lecture Theatre (Chemistry)
Posters:	North Cloisters (UCL)
Conference Meal:	Jeremy Bentham Room (UCL)
Refreshments:	Nyholm Room (Chemistry)



The first Polar Solids Meeting was held at UCL Chemistry Department thirty years ago. Now part of the Royal Society of Chemistry Solid State Group programme, this year's Christmas meeting returns to UCL with local accommodation at Passfield Hall.



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## Invited Speakers

C. Serre	Institut Lavoisier, Versailles
C.P. Grey	University of Cambridge
A.V. Chadwick	University of Kent
D.J. Willock	University of Cardiff
C.F. Hirjibehedin	London Centre for Nanotechnology

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The organising committee would like to thank Crispin Cooper for his time spent addressing delegate queries, and helping us with the general administration required in organising this year's Christmas meeting, in particular, collating registration forms.

## Porous MOFs for biomedical and thin films related applications

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MOFs or Metal Organic Frameworks, are the latest class of porous crystalline solids. They possess a tunable composition and pore size associated with the presence of both inorganic and organic species within their frameworks that make them suitable for many potential applications such as gas storage, separation or catalysis.<sup>1</sup> Recently, it has been shown that some MOFs could be used in biomedicine for the controlled delivery of model drugs (Ibuprofen)<sup>2</sup>. This approach has been extended recently to nanoparticles of porous iron carboxylates for the controlled release of anticancer or anti-retroviral drugs of high interest.<sup>3</sup> These particles exhibit imaging properties while they are non toxic and biodegradable. MOFs that possess coordinatively unsaturated metal sites are of interest for the delivery of nitric oxide. Finally, MOFs based on bioactive linkers might be considered as an alternative method for the controlled delivery of drugs.<sup>4,5</sup>

Elaboration of thin films of MOFs has been also recently studied due to the enormous prospects in nanotechnology based applications such as in membranes, responsive or catalytic coatings, sensors and other related nanodevices.<sup>1</sup> We have prepared thin films of MOFs of high optical quality of several MOFs of interest, using the chemical solution deposition of preformed nanoparticles (NPs) on a bare surface. We present here their elaboration by dip-coating thin films of several rigid or flexible MOFs.<sup>2,3,4</sup> Vapors adsorption of water or alcohols, has been finally used to evaluate the response of the resulting thin films through environmental ellipsometric porosimetry. This showed that these systems exhibit a hierarchical porosity and a reversible thickness increase upon water adsorption as well as a selective behaviour in the presence of mixtures of water and alcohols.

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## 3D Microbatteries: Conformal deposition of battery materials on porous 3D substrates

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There has been much recent interest in the 3D microbattery concept; the 3D concept combines the high rate performance of the thin film battery with the energy performance of a thick film battery without the need for large footprint areas, making it more suitable for microscale or MEMS applications (1-2). The majority of these designs are based on the lithium-ion system, and common to this is the need to have two closely spaced electrodes separated by a thin electrolyte layer. In this paper we will describe the conformal deposition of Li-ion battery electrodes onto 3D substrates.

Two approaches have been taken for the deposition of electrodes onto a reticulated vitreous carbon substrate (Figure 1a), which acts as our 3D microbattery current collector. The first is to electrodeposit  $\text{MnO}_2$  (Figure 1b) from a solution containing 0.3 M  $\text{MnSO}_4$  and 0.3 M  $\text{H}_2\text{SO}_4$ . This has been calibrated and controlled such that conformal layers of between 0.5 and 10  $\mu\text{m}$  can be produced. A second method is to immerse the foams in an ink containing a battery material ( $\text{LiFePO}_4$ ) with binder and conductive additive. The excess ink is then removed by spin coating and a thin layer of composite material remains attached to the foam struts (Figure 1c). Repetition of this dip spin coating step leads to thicker conformally coated foams.

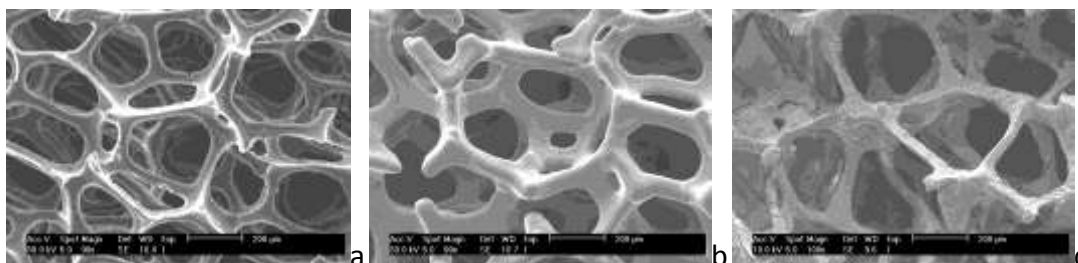


Figure 1. SEM images of RVC substrate (a), EMD (b) and  $\text{LiFePO}_4$  composite electrode (c) conformally coated over the whole RVC structure.

Results will show structural and electrochemical characterisation of these materials indicating the capacity per footprint area improvements possible with these structures. In some cases as much as a 50 x improvement is seen with capacities of  $10 \text{ mA h cm}^{-2}$ .

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## Structural Investigations of Disordered Metal Oxides

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Many materials exhibit some degree of structural disorder ranging from the completely amorphous, with order only on the shortest length scales, to disordered crystals which exhibit local deviations from the average structure. Full characterisation of such materials is a challenge which requires the use of techniques that can probe their local structure.

We report the structural characterisation of a variety of disordered metal oxides using a combination of approaches, particularly total neutron scattering. As well as using traditional Rietveld refinement against diffraction data to determine the average structure, we also apply the analogous technique of Pair Distribution Function (PDF) analysis<sup>1</sup> to the real-space data to examine the local structure. Examples to be presented include gallium oxide and bismuth-doped cerium oxide.

Several of the polymorphs of gallium oxide, Ga<sub>2</sub>O<sub>3</sub>, are disordered. Our work has shown that the structure of the cubic defect-spinel  $\gamma$ -Ga<sub>2</sub>O<sub>3</sub> includes four partially occupied Ga sites. The distribution of Ga across these sites has been studied by PDF analysis and Reverse Monte Carlo (RMC) modelling.

A series of bismuth-doped cerium oxides, Ce<sub>1-x</sub>Bi<sub>x</sub>O<sub>2-(x/2)</sub> with  $x \leq 0.6$ , have been prepared hydrothermally.<sup>2</sup> They have the average cubic fluorite structure with significant local distortion of the Bi coordination environment similar to that found for  $\gamma$ -Bi<sub>2</sub>O<sub>3</sub>.<sup>3</sup> Similar analysis is currently being carried out on cerium based pyrochlores. It is hoped that these methods will help to understand the materials' potential for catalytic behavior.

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# New directions in the microwave synthesis of inorganic materials; complex carbides and time-resolved reaction probes

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Conventional synthesis of solid state materials is time and energy intensive. Microwave (MW) synthesis is emerging as a viable alternative, allowing access to new metastable materials and offering synthetic routes that are considerably quicker than conventional methods. There are, however, considerable barriers to overcome.

Ex-situ analysis of the products of MW reactions allows characterisation of the materials formed, but gives little insight into reaction mechanism. Ultimately, in-situ reaction probes are needed to gain this additional information. For this purpose, we are developing a bespoke MW reactor for use with the POLARIS diffractometer at the ISIS neutron source (Fig.1), which will enable us to study reactions in-situ using high intensity, time-resolved neutron diffraction. We will present details of the development of our reactor and discuss future experiments to probe structure, bonding, kinetics and dynamics in a wide range of MW reactions for the first time.

Carbon-containing materials are attractive candidates for MWs due to the strong interaction of carbon with a MW field, resulting in rapid temperature increases and fast reaction times. Transition metal (TM) carbides possess properties including high melting points, hardness, toughness and resistance to oxidation/ reduction, which results in their main applications as cutting tools and wear-resistant parts. There is also some interest in TM carbides for catalytic applications.<sup>1</sup> Many TM carbides superconduct, and their transition temperatures ( $T_c$ ) often exhibit a strong dependency on both metal and carbon stoichiometry.<sup>2-4</sup> Previous work resulted in the successful MW synthesis of WC, Mo<sub>2</sub>C and Nb<sub>1-x</sub>Ta<sub>x</sub>C<sup>3,5</sup> and we have subsequently investigated other ternary carbides. We present here our initial results of the synthesis of three solid solutions, Nb<sub>1-x</sub>Mo<sub>x</sub>C (Fig. 2), Ta<sub>1-x</sub>Mo<sub>x</sub>C and Mo<sub>1-x</sub>W<sub>x</sub>C ( $x = 0.4- 0.8$ ), from reaction of appropriate TM oxides with graphite in a multimode MW cavity, and a preliminary study of superconductivity in these ternary TM carbides.

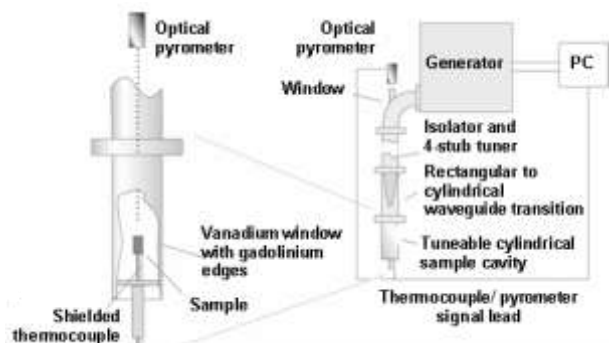


Fig.1 Basis of design for the reactor to be used on POLARIS

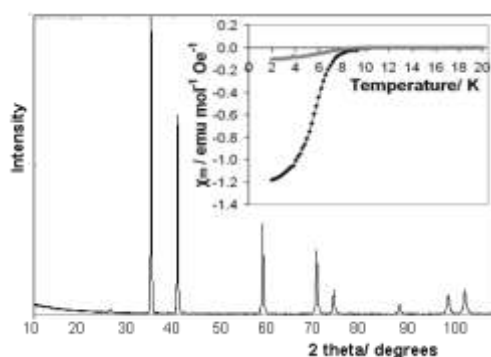


Fig 2. PXD and magnetic data for cubic Nb<sub>0.65</sub>Mo<sub>0.35</sub>C

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## Following Function in Real Time: New NMR Methods for Studying Structure and Dynamics in Batteries and Fuel Cell Materials

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The application of new Nuclear Magnetic Resonance (NMR) and X-ray approaches to correlate structure and dynamics with function in materials lithium-ion batteries and solid oxide fuel cells will be described. A particular focus is the development of methodology to allow these systems to be investigated *in-situ*, i.e., under realistic operating conditions. This allows processes to be captured, which are very difficult to detect directly by *ex-situ* methods. For example, we can detect side reactions involving the electrolyte and the electrode materials, and processes that occur during extremely fast charging and discharging. The approach will be demonstrated for the anode material silicon. Lithium-ion batteries (LIBs) containing silicon have been the subject of much recent investigation, because of the extremely large gravimetric and volumetric capacity of this anode material. This material undergoes a crystalline-to-amorphous phase transition on electrochemical Li insertion into crystalline Si, during the first discharge, hindering attempts to link structure in these systems with electrochemical performance. We apply a combination of static, *in-situ* and magic angle sample spinning, *ex-situ*  $^7\text{Li}$  and  $^{29}\text{Si}$  nuclear magnetic resonance and pair distribution function analysis studies to investigate the changes in local structure that occur in the actual working LIB. The first discharge occurs via the formation of isolated Si ions and smaller Si-Si clusters embedded in a Li-ion matrix; the latter are broken apart at the end of the discharge forming isolated Si ions. In a second example, we illustrate the use of NMR to investigate the nature of the defects in materials that have been proposed for use as electrolytes that operate via either oxygen-ion or protonic conduction in solid oxide fuel cells. For example,  $\text{BaZrO}_3$  or  $\text{BaSnO}_3$  can be doped with  $\text{Y}^{3+}$  to create oxygen vacancies. These vacancies can be filled with  $\text{H}_2\text{O}$ , the water molecules dissociating to form mobile ions that contribute to the long-range ionic transport in these systems. NMR experiments are used to examine the local structure, the locations of the vacancies and how this affects protonic/oxygen ion motion in these systems.



## Novel Electrode Materials for Fuel Cells

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Due to the continuing problems regarding increasing production of greenhouse gases and the depletion of fossil fuels there is a need for more efficient power generating technologies. Fuel cells offer a solution to this problem, with their improved efficiencies compared to traditional means of electricity generation. In terms of stationary power applications, solid oxide fuel cells (operating between 500-1000°C) are being targeted due to their greater fuel flexibility compared to low temperature PEM fuel cells.

In terms of the cathode for SOFCs, the structure-type that has generated the most interest is the perovskite, due to the high ionic conductivity and electronic conductivity, as well as catalytic potential for oxygen reduction, of transition metal containing systems with this structure. Some examples include  $\text{La}_{1-x}\text{Sr}_x\text{Co}_{1-y}\text{Fe}_y\text{O}_{3-\delta}$  (LSCF),  $\text{La}_{1-x}\text{Sr}_x\text{FeO}_{3-\delta}$  (LSF) and  $\text{La}_{1-x}\text{Sr}_x\text{MnO}_{3-\delta}$  (LSM) [1-3], with cobalt containing systems showing the best mixed (ionic plus electronic) conducting properties. Traditionally doping strategies to optimise the properties of these perovskite systems, have involved the introduction of aliovalent cation dopants with similar sizes; e.g. Sr for La. Recently we have been investigating an alternative doping strategy for solid oxide fuel cell materials, namely the incorporation of tetrahedral oxyanions such as sulphate, phosphate, and silicate, and in this work we present initial studies investigating the effect of such dopants on the structure and conductivity of  $\text{SrMnO}_3$  and  $\text{SrCoO}_3$ , comparing the results to conventional doping studies [4, 5].

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# Modelling and NMR Studies of Defect Sites and Conduction Pathways in Apatite-type Electrolytes for Solid Oxide Fuel Cells

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The viability of low carbon energy technologies such as fuel cells is crucially dependent on the fundamental properties of the component materials. Apatite-type silicates/germanates are attracting considerable interest as new oxide ion conducting electrolytes for use in solid oxide fuel cells [1]. However, a complete atomic-scale understanding of their local structural and conduction properties is still lacking. Here, we utilise a combined spectroscopic and computational approach to elucidate the defect characteristics and conductivity mechanisms in the apatite germanate  $\text{La}_8\text{Y}_2\text{Ge}_6\text{O}_{27}$ , which exhibits high oxide-ion conductivity and high oxygen excess. Through modelling and solid state  $^{17}\text{O}$  NMR data we show that the interstitial oxide ion defects are associated with the Ge leading to the formation of five coordinate Ge. In addition, we show that the migration of these defects occurs via cooperative mechanisms involving the framework tetrahedral. Recent studies of water incorporation and local O-H configurations in Si and Ge-apatites are also discussed [2], which extends previous work on gallate ionic conductors [3].

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# Interfacial Strain Effects in Oxide Ion Conducting Multilayer Heterostructures: Undoped Ceria/Ionic Conductor Systems

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The study of thin film multilayer oxide heterostructures has been of significant interest over the past few years due to several publications reporting the ability to manipulate ionic conductivity at heterointerfaces. Further study of this effect could be of great significance in the development of materials solid oxide fuel cell and oxygen separation membrane applications.

In this work we investigate the behaviour of several multilayer systems with alternating insulating ( $\text{CeO}_2$ ) and oxide ion conducting layers ( $\text{Ce}_{1-x}\text{R}_x\text{O}_{2-x/2}$  ( $\text{R} = \text{Sm}, \text{Nd}$  or  $\text{Y}$ ) or YSZ (8 mol%  $\text{Y}_2\text{O}_3$ )). All samples were grown by pulsed laser deposition on (100) oriented single crystal MgO substrates and grew in a cube on cube configuration. Interfacial density was increased for each system while maintaining an overall thickness throughout to allow separation of interfacial behaviour. Conducting layers of doped ceria and YSZ were chosen to vary the lattice misfit between -0.75% to +3.7%.

The conductivity behaviour of these samples was measured using impedance spectroscopy allowing correlation of sample conductivity to both interface density and misfit. The nature of the charge carrier has been investigated using isotopic exchange and SIMS and the structure, by X-ray diffraction and TEM.

## Thirty Years Of The Solid State Group

Alan Chadwick

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In December 1980 an informal meeting was held at University College, London to consider the status of solid state chemistry in the UK. This resulted in the formation of the *Polar Solids Group*, which through a number of mergers and changes of name is now the present *Solid State Chemistry Group of the Royal Society of Chemistry*. This talk will present a light-hearted review of the history of the Group and the growth of solid state chemistry and materials chemistry from niche areas in the 1980s to major pillars of current chemical research. The review will include coverage of the significant meetings, events and people that were instrumental in developing these areas in the UK. The talk will conclude with a forward look to possible future developments in solid state chemistry.

## Heterogeneous oxidation catalysts surface

David Willock

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In this presentation we will look at the use of periodic DFT methods for the simulation of catalyst surfaces. We will focus on oxidation chemistry using oxides and metal particles supported on oxides. To describe transition metal oxides some approach beyond gradient corrected DFT or Hartree Fock theory is required. We have used the DFT+U approach to study the defective surface of  $\text{MoO}_3$ , adsorption of dioxygen and C-H bond activation in methane as an example and show how the Hubbard U parameter leads to electron localisation on the reduced surface.

This method can also be applied to metal oxides with magnetic ordering, such as  $\text{Fe}_2\text{O}_3$ . Recent experimental work on Au supported by iron oxide has shown high activity for the CO oxidation reaction. The early time products of this reaction have been analysed using a temporal analysis of products reactor (TAP) with the unexpected observation that some of the CO dissociates over the catalyst. We use DFT+U calculations to look at the adsorption of  $\text{O}_2$  at the metal/oxide interface and show that CO dissociation is possible if it occurs at the same time as  $\text{O}_2$  bond scission.

# Molecular modelling of the adsorption of uracil molecules on gold surfaces

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Supramolecular films on surfaces are of increasing interest owing to their applications in functionalized surface-based technologies. These structures can interact through covalent bonds to the surface atoms but the assembled films are organised by noncovalent interactions, i.e. hydrogen-bonds and van der Waals forces.

We have focused on the DNA/RNA bases and their noncovalent base-pairing interactions to gain structural and morphological information on the possible 2D mismatch pairings between bases, which can sometimes lead to tumours. Our work aims to acquire a deeper understanding of the ordering and functionality of complex structures of biological interest on metal surfaces.

Here we present the results of our plane-wave Density Functional Theory calculations of the adsorption of uracil on two surfaces of gold, Au(100) and Au(111). The differences and similarities of adsorption and assembly modes between the surfaces help our understanding of the role of the

substrate in comparison to the lateral noncovalent intermolecular interactions. A systematic analysis of the adsorption of uracil molecules on Au(100) and Au(111) has been undertaken. In Fig. 1 we highlight the preferred adsorption mode of enol uracil on Au(100). Results are compared with previous STM findings<sup>1</sup>.

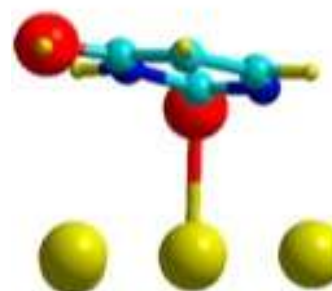


Figure 1

## References

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# An *ab initio* Description of the Bulk and Surface Structures of UO<sub>2</sub> using GGA+U and Occupation Matrix Control

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The study of the bulk and surface properties of UO<sub>2</sub> has been a major research topic for at least the past 70 years, and interest in the structure, stability and catalytic behaviour of the surfaces of this material has greatly intensified in the past decade<sup>1</sup>. Nonetheless, in spite of numerous attempts a sound first-principles description of the bulk and surface properties of this important material has proven elusive.

In this work we demonstrate the major difficulties that have been encountered in the search for an accurate *ab initio* description of UO<sub>2</sub>. It is well known that the correlation effects associated with the two 5*f*-orbital electrons in the outer shell of U<sup>4+</sup> leads to the erroneous prediction of the ground state electronic and magnetic behaviour; it is also well known that these errors can be *prima facie* corrected by the judicious application of a Hubbard-like U term. Recently, it has been pointed out<sup>2</sup> that this treatment leads to the problematic prediction of metastable states, where during electronic relaxation simulations the 5*f* electrons become ‘trapped’ in states which do not correspond to the true ground state of the system. This has been shown to have a particularly strong effect with regards to the calculation of defect energies, where large errors have been noted.

In this work we extend this treatment to the surfaces of UO<sub>2</sub>. The sole *ab initio* study of UO<sub>2</sub> surfaces<sup>3</sup> present in the literature did not consider the 5*f* electron correlations, and as such incorrectly predicted UO<sub>2</sub> to be metallic. We demonstrate that while the application of the U parameter corrects this, it is still not possible to converge the surface energies of any of the three most commonly observed surfaces, namely the (111), (110) and (100). However, by combining the monitoring of orbital occupancies and the Hubbard-like term the difficulties in the description of the surfaces of UO<sub>2</sub> are overcome. We demonstrate a novel methodology which determines the ground state for slabs of increasing thicknesses, until convergence of the surface energy is ensured. The resulting (100), (110) and (111) surfaces are energetically and structurally in excellent agreement with those determined from experimental and atomistic-based theoretical studies.

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# The Interesting Chemistry of some Thallium Containing Oxides: An Explanation and a Prediction.

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The ground state electronic structure of thallic oxide ( $\text{Tl}_2\text{O}_3$ ) has remained contentious for decades. It has been known for some time that  $\text{Tl}_2\text{O}_3$  displays metallic conductivity but there has been no consensus as to whether this is an intrinsic property of the stoichiometric phase, or arises from oxygen deficiency in  $\text{Tl}_2\text{O}_{3-x}$ . Recent GGA-DFT calculations predict  $\text{Tl}_2\text{O}_3$  to be a semi-metal, possessing a single band that disperses across the Fermi energy, with the Fermi level sitting near the top of the O  $2p$  valence band. XPS experiments, however, report that the Fermi level lies about 1.1 eV above the main valence band edge. Optical absorption experiments add another level of complexity to this puzzle, finding optical band gaps of  $\sim 2.5\text{--}2.7$  eV. In this presentation we use GGA-DFT and the screened hybrid density functional HSE06 to explain these reported inconsistencies and outline the correct ground state electronic structure of  $\text{Tl}_2\text{O}_3$ . We also use the insights gained from this study, to predict a novel thallium containing transparent conducting oxide, which shows the greatest potential thus far for bi-polar TCO applications.



# The impact of the local environment on the Kondo screening of a high-spin atom

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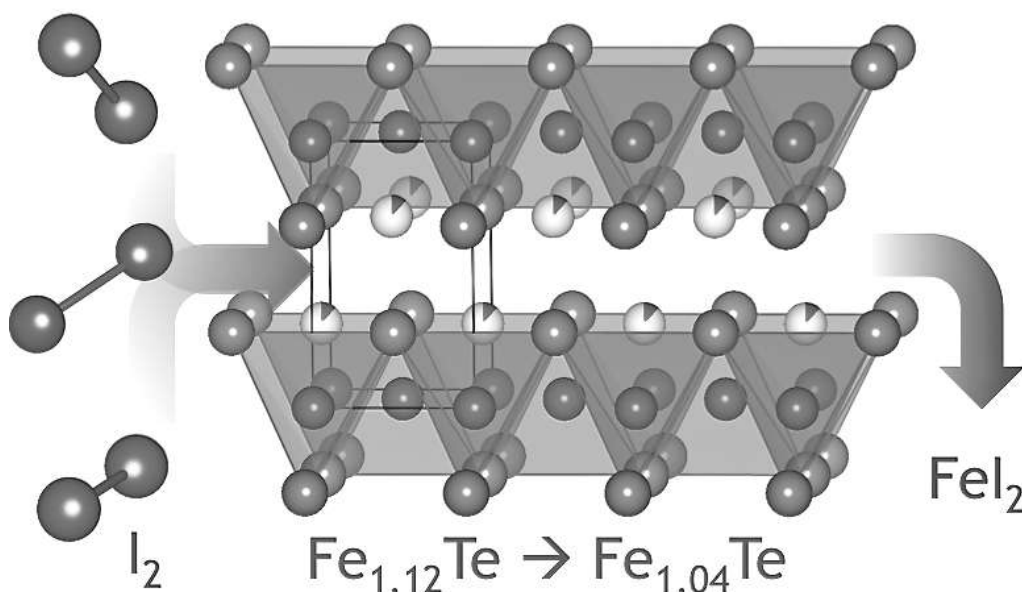
Kondo screening is a many-body phenomenon arising from the interaction between a localized magnetic moment and the conduction electrons in a metal. Spin 1/2 Kondo systems have been investigated extensively in theory and experiments. However the magnetic atoms that give rise to the Kondo effect in metals often have a larger spin, which makes the properties of the system more complex. Using a low-temperature scanning tunneling microscope, we explore the Kondo effect of individual high-spin magnetic atoms on surfaces. Using a combination of elastic and inelastic tunneling spectroscopy, we determine the spin of the atom and explore its impact on the Kondo resonance. We demonstrate that the local magnetic anisotropy plays a decisive role in the physics of Kondo screening. In addition, we can tune the Kondo resonance through other parameters, such as coupling to a neighboring unscreened spin and a magnetic field.

# The Role of Interstitial Iron in the Magnetism and Superconductivity of Iron Chalcogenides

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In 2008, the field of superconductivity received one of its largest boosts since the cuprates with the arrival of the iron-based superconductors. While the first compounds were mostly oxypnictides and pnictides such as  $\text{LaO}_{1-x}\text{F}_x\text{FeAs}$  and  $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ , the number of members expanded with the discovery of superconductivity in iron chalcogenides. For the latter compounds, we discuss the role that the interstitial iron atoms play in determining the type of magnetic ordering that takes place, and whether superconductivity is expressed at all. First, we present neutron scattering measurements of the phases  $\text{Fe}_{1+x}\text{Te}$  for  $x = 0.07, 0.12,$  and  $0.18$ . The  $x$  in  $\text{Fe}_{1+x}\text{Te}$  corresponds to interstitial iron located between the two-dimensional sheets of edge-sharing  $\text{FeTe}_4$  tetrahedra (See Figure). The low energy spectrum (0.5 meV to 10 meV) of the magnetic excitations will be presented as well as neutron polarized diffraction experiments that detail the nature of the magnetic ordering. Second, we present a *chemie douce* technique that topotactically de-intercalates the interstitial iron from the lattice. Our analysis of the neutron inelastic data of de-intercalated samples indicates that paramagnetism from this interstitial iron is detrimental to superconducting properties, supporting our magnetization measurements that show how the superconducting volume fraction is indeed increased as the amount of interstitial iron is removed. Diffraction results detailing changes in key structural parameters and magnetic ordering will also be presented.



## Structure – property relationships in quaternary manganese pnictides $AMnPnF$ ( $A = Ba, Sr, Pn = P, As, Sb$ )

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The discovery of superconductivity in iron pnictides has led to an enormous interest in layered materials adopting the tetragonal ZrCuSiAs-type structure. The “1111”  $R_EFeAsO$  parent materials are poor metals showing magnetic instabilities at low temperatures. Numerous iron based compounds have been studied, but also isostructural  $R_ET_MPnO$  materials ( $R_E =$  rare earth;  $T_M =$  transition metal;  $Pn =$  pnictide) have been investigated in order to understand the interplay of structure, magnetism and superconductivity. Although their physical properties depend on the number of d-electrons on  $T_M$  – ranging from non-magnetic through to ferromagnetic and antiferromagnetic ( $T_M = Zn, Co, Mn$ , respectively) – they can be tuned by chemical substitution in the insulating  $[R_EO]$  layer.

Our research focused on the investigation of related manganese fluoride compounds  $AMnPnF$  ( $A = Sr, Ba; Pn = P, As, Sb$ ), whose electronic/ magnetic response is expected to be different from the superconducting Fe- and Ni- materials (half-filled pseudo closed shell –  $3d^5$  vs even number of d-electrons). Variable temperature synchrotron X-ray and neutron powder diffraction, resistivity and magnetic measurements were employed to carefully map the electronic, magnetic and structural phase diagrams. Substitution of the pnictide enhances the magnitude of the  $Mn^{2+}$  ( $S = 5/2$ ) moments and the electrical conductivity whereas replacement of the alkaline metal ( $Sr \rightarrow Ba$ ) alters the physical properties drastically whilst maintaining the ZrCuSiAs structure.

## Rare Earth Substituted Multiferroic BiFeO<sub>3</sub>

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BiFeO<sub>3</sub> is one of the most widely studied multiferroic materials because of its magnetoelectric properties (i.e. ferroelectric, with a high Curie temperature,  $T_C \sim 810 - 830$  °C, and antiferromagnetic with  $T_N \sim 370$  °C)<sup>1</sup>. The study and application of BiFeO<sub>3</sub> is hindered by its thermal metastability and overriding electrical conduction due to non-stoichiometry<sup>2</sup>. One common approach to improve the properties is by substitution of the volatile Bi<sup>3+</sup>. In this case we dope BiFeO<sub>3</sub> with lanthanum (Bi<sub>1-x</sub>La<sub>x</sub>FeO<sub>3</sub>) and neodymium (Bi<sub>1-y</sub>Nd<sub>y</sub>FeO<sub>3</sub>). This results in improved stability of the perovskite phase.

We have investigated structural transitions as a function of temperature and degree of doping using a number of different techniques including XRD and electrical impedance spectroscopy. We propose a series of transitions from R3c - Imma ( $x = 0.3$ ) - Pbnm ( $x \leq 50$ ) within the lanthanum doped system (BLFO). In contrast the neodymium doped system shows the existence of a Pbam phase (R3c - Pbam - Pbnm). Electrical characterisation of the materials are also discussed.

<sup>1</sup>G. Catalan & J.F Scott, *Adv. Mater.*, **21** (24), 2463, 2009.

<sup>2</sup> W. Eerenstein, F.D. Morrison, J. Dho, M.G. Blamire, J.F. Scott & N.D. Mathur, *Science*, **307** (5713), 1203a, 2005.

## Insulator-metal transitions in vanadium oxides

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### Abstract

Vanadium oxide materials have received considerable attention not only for their potential uses in a number of technological applications, but also because of the interesting physics associated with the metal-insulator transitions displayed by a number of these oxides. In this talk, I will describe several synthetic routes for the preparation of vanadium oxide nanostructures and discuss our observations of the structure, morphology and electrical properties of these materials. The electrical property changes in rutile  $\text{VO}_2$  raise a number of interesting questions, particularly the structural nature of the material at the transition temperature. There has been a lot of confusion about structural changes at this famous transition because of a lack of direct information on the local variation of the atomic positions. I will

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show synchrotron x-ray total scattering studies and reverse Monte Carlo simulations of the structural changes occurring in rutile  $\text{VO}_2$  as it goes through its metal-insulator transition. By adopting these methods of structural analysis, we have shown that there is no evidence for intermediates upon heating up the material, nor fleeting signatures of the metallic phase at room temperature, as hinted in some of previous studies. The findings are vital to better understanding the nature of the transition.

## Posters

Dr Mark S D Read	AWE	An ab initio Description of the Bulk and Surface Structures of $\text{UO}_2$ using GGA+U and Occupation Matrix Control
Miss Sarah J Ewing	Heriot Watt University	Solvothermal Synthesis of Indium Selenides
Dr Monica Burriel	Imperial College	Oxygen diffusion and surface exchange in $\text{PrBaCo}_2\text{O}_{5+x}$ layered cobaltite
Mr Poh Shing Ong	Imperial College	Synthesis of Ca and Sr doped GDC solid solutions by oxalate co-precipitation technique and its characterizations
Ms Nasima Kanwal	Queen Mary London	Phosphate Based Glasses for Potential Use as Glass Ionomer Cements for Bone Cement Applications.
Prof. Louis F J Piper	SUNY Binghamton	Soft X-ray Spectroscopy of Oxychalcogenides: Relating Electronic Structure with p-type Conductivity
Dr Elaine A Moore	The Open University	The Effect of Doping on the Properties and Structure of Perovskites.
Dr Jeremy P Allen	Trinity College Dublin	The Mixed Valence of AgO: The Failure of GGA and the success of HSE
Mr Kalle M Korpela	Trinity College Dublin	Electronic Structure and stability of ternary Cu-based delafossite transparent conducting oxides
Dr Aron Walsh	UCL	Crystal Structure and Defect Reactions in the Kesterite Solar Cell Absorber $\text{Cu}_2\text{ZnSnS}_4$ (CZTS): Theoretical insights.
Miss Hsin-Yi Tiffany Chen	UCL	trans-Fe(ii)(H) <sub>2</sub> (DIPHOSPHINE)(DIAMINE) Complexes as alternative catalysts for asymmetric hydrogenation of ketones? A DFT study.
Dr Jorg Saßmannshausen	UCL	DFT calculations of a multi-metallic complex with a planar $\text{Cu}_4\text{OH}$ Motif
Mr Grahame R Gardiner	University of Bath	Defects and Ion Migration in Phosphate and Fluoro-sulphate Materials for Lithium Batteries
Mr Alaric D Smith	University of Birmingham	Oxyanion Doping into Solid Oxide Fuel Cell Electrolytes
Mr J. Felix Shin	University of Birmingham	Oxyanion doping in perovskite-type fast ion conductors: preparation of new phases and enhancement of oxide ion/proton conductivity and $\text{CO}_2$ stability
Dr Derek S Middlemiss	University of Cambridge	Combining Experimental and Theoretical Paramagnetic NMR Spectroscopy for the Characterisation of Li-ion Battery Cathodes
Dr Paul Saines	University of Cambridge	Atomic and Magnetic Structures of the Antiferromagnetic Mn Succinate Hybrid Framework, $\text{Mn}(\text{C}_4\text{H}_4\text{O}_4)$
Dr Emma E McCabe	University of Durham	New iron and manganese oxyselenides: structural and physical characterisation

Dr Takeshi Nakagawa	University of Edinburgh	The temperature and pressure dependence of structural properties of the ternary transition metal fluoride $K_{0.9}CrF_3$
Miss Jamie B Gallagher	University of Glasgow	Sub-minute growth of nanostructured, monodisperse titanium dioxide microspheres; synthetic control, structure and properties.
Miss Nuria Tapia Ruiz	University of Glasgow	Novel microwave synthesis of $Li_{3-x}M_xN$ (M=Cu, Co, Ni) for their use as anodes in Li-ion batteries.
Mr James M Hanlon	University of Glasgow	New Nanostructured Hydrogen Release Systems
Dr David J Cooke	University of Huddersfield	Atomistic Simulation of Thorium Molten Salts
Miss Amy Monnington	University of Huddersfield	Atomistic simulation of cobalt doped iron oxides
Dr Serena A Corr	University of Kent	Real-space investigation of the insulator-metal transition in vanadium dioxide
Dr Rapela R Maphanga	University of Limpopo	Atomistic Simulation Studies of Electrolytic Manganese Sioxide
Dr Giorgio Lanzani	University of Oulu	The Aquatic Chmeistry of Aluminium: Kinetics and Dynamics
Mr Benjamin M Gray	University of Southampton	Surface Modification of Titanium Nitride for Electrochemical Applications: An X-ray Photoelectron Spectroscopy Study.
Mr Syed Shah	University of Southampton	Metal / Silicon Nitride Composite Structures
Dr Enrique Ruiz-Trejo	University of St Andrews	Electrochemichal Characterization of Proton Conducting Membranes
Dr Finlay D Morrison	University of St Andrews	Dipole stability and dynamics in tetragonal tungsten bronze dielectrics
Dr Maarten C Verbraeken	University of St Andrews	Structure and electrical properties of barium hydride
Dr Richard J Goff	University of St Andrews	A Search for New Multiferroic Fluorides
Mr Lewis J Downie	University of St Andrews	Structural, magnetic and electronic studies of hexagonal $RFeO_3$ (where R = Y and Yb)
Sarah A Turp	University of St Andrews	$BaTiO_3$ based lead-free piezoelectronics
Miss Oonagh M Collins	University of Strathclyde	Magnetic Dilution in Magnetoresistive Perovskites; Cation Doping in $Ba_2FeMoO_6$
Mr Peer I Cowin	University of Strathclyde	Development of Novel Anode Materials for Intermediate Temperature Solid Oxide Fuel Cells

Dr Peter W Dunne	University of Warwick	Synthesis of hybrid ceria/mesoporous silica nanocomposites
Miss Alexis S Munn	University of Warwick	An Investigation into the different stages of “breathing” in MIL-53-type MOFs
Mr Robin D Fisher	University of Warwick	New synthetic methods to improve the water resistance of gypsum
Mr Paul J Weaver	University of Bath	Defect, ion transport and electronic properties of infinitely layered SrFeO <sub>2</sub> atomistic simulation and DFT studies
Miss Rebecca K Yue	University of Durham	Recent work to be revealed
Dr David F Plant	AWE	Recent work to be revealed
Ricardo Grau-Crespo	UCL	Ab initio thermodynamics of hydrogen vacancies in pure and Li-doped magnesium hydride
Sam Alexander	UCL	A combinatorial nano precursor route for direct solid state chemistry; discovery and electronic properties of new iron doped lanthanum nickelates up to La <sub>4</sub> Ni <sub>2.1</sub> Fe <sub>0.9</sub> O <sub>10-β</sub>
M A Mehlape	University of Limpopo	Computer simulation of mineral sulphide
Cristina I Olariu	University of Liverpool	Multifunctional nanoparticles for healthcare applications
M Tsiamtsouri	University of Liverpool	Langasites as interstitial oxide ion conductors for SOFC electrolytes
Matthew S Dyer	University of Liverpool	Understanding Photocatalytic Activity in CaCu <sub>3</sub> Ti <sub>4</sub> O <sub>12</sub>
Alexey Ganin	University of Liverpool	Two faces of cubic Cs <sub>3</sub> C <sub>60</sub>
R. Sayers	University of Liverpool	Electrochemical performance of layered perovskites for intermediate temperature solid oxide fuel cells
Jesse Dufton	University of Bath	Computational Investigation of Absorber Materials for Inorganic Solar Cells



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# RSC Solid State Chemistry Group

## 30<sup>th</sup> Anniversary Christmas Meeting

### Monday 20<sup>th</sup> December 2010

**1:30 Welcome**

**1:40** C. Serre – Porous MOFs for biomedical and thin films related applications

**2:20** M. Roberts - 3D microbatteries: Conformal deposition of battery materials on porous 3D substrates

**2:40** H.Y. Playford - Structural investigations of disordered metal oxides

**3:00** H.J. Kitchen - New directions in the microwave synthesis of inorganic materials; complex carbides and time-resolved reaction probes

**3:20 Tea break**

**3:50** C. Grey – Following function in real time: New NMR methods for studying structure and dynamics in batteries and fuel cell materials

**4:30** C.A. Hancock - Novel electrode materials for fuel cells

**4:50** P.M. Panchmatia - Modelling and NMR studies of defect sites and conduction pathways in apatite-type electrolytes for solid oxide fuel cells

**5:10** S.N. Cook - Interfacial strain effects in oxide ion conducting multilayer heterostructures: undoped Ceria/ionic conductor systems

**5:30** A.V. Chadwick – Thirty years of the Solid State Group

**6:10 AGM**

**6:30 Posters**

**7:30 Conference Meal**

### Tuesday 21<sup>st</sup> December 2010

**9:00** D. Willock – Heterogeneous oxidation catalysts surface

**9:40** S. Irrera - Molecular modelling of the adsorption of uracil molecules on gold surfaces

**10:00** A.J. Devey - An ab initio description of the bulk and surface structures of UO<sub>2</sub> using GGA+U and occupation matrix control

**10:20** D.O. Scanlon - The interesting chemistry of some thallium containing oxides: an explanation and a prediction

**10:40 Coffee**

**11:10** C. Hirjibehedin – The impact of local environment on Kondo screening of a high-spin atom

**11:50** E.E. Rodriguez - The role of interstitial Fe in the magnetism and superconductivity of iron chalcogenides

**12:10** C. Drathen - Structure – property relationships in quaternary manganese pnictides AMnPnF (A = Ba, Sr, Pn = P, As, Sb)

**12:30** C.M. Kavanagh - Rare earth substituted multiferroic BiFeO<sub>3</sub>

**12:50** S.A. Corr – Real-space investigation of the insulator-metal transition in vanadium dioxide

**13:10 Wrap-up**