Ab initio simulations of ferroelectric PbTiO$_{3}$ on SrTiO$_3$ substrates: tilted flux closure
Jack Baker (UCL)

We present ab initio calculations on thin films of PbTiO$_{3}$ mounted on SrTiO$_3$ substrates. We utilise fully self-consistent DFT to study systems of extended size ($\leq$ 2088 atoms) using the new multisite support function method as implemented in the CONQUEST code. We explore the structure and energetics of the ferroelectric flux closure domains in films up to 36nm thick. We treat explicitly the SrTiO$_3$ substrate and the c(2x2) PbTiO$_{3}$ surface reconstruction. We find domain patterns with anti-phase tilts in the [001] direction possessing a periodic shift in the domain wall chiral centre.

Effect of Exchange-correlation functional on spin-admixture parameter calculated from first principles
Uday Chopra (Johannes Gutenberg University)

Organic semiconductors (OSC) are known to have a small spin-orbit coupling (SOC) and this has strong implications in their spintronic properties. It has been shown that SOC can be characterised by mixing of up- and down-spin states and is expressed by the spin-admixture parameter, γ2[1]. This parameter governs the probability of a spinflipping as the charge hops between different sites in the OSC. Since for most OSC, transport is described by hopping mechanism, the spinrelaxation time is very sensitive to γ2 therefore it becomes important to determine the parameter with high accuracy. We present a method for calculation of spin-admixture in organic semiconductors from firstprinciples on the level of Density Functional Theory. In this work, we use a methodical procedure to obtain precise values of γ2 and demonstrate the effect of exchange-correlation functional on the parameter. Moreover, we generalise this approach under the Unrestricted DFT. We also and that γ2, strongly depends on the delocalization error of the functional and tends to decrease as the functional becomes more localized.

Edge Distribution of a 1-D Bose Gas
Michael Clark (Birmingham)

We consider the probability distribution of the last particle in a 1-D harmonically trapped Bose gas. A phenomenon related to the emptiness formation probability. By considering two different interaction regimes we investigate how this distribution changes with interaction strength and hypothesize a link between the two regimes.

Gas Hydrates and HCNO under High Pressure
Lewis Conway (Edinburgh)

Icy planets and moons such as Neptune, Uranus, Titan and an significant proportion of exoplanets contain mixtures H20, NH3 and CH4, not necessarily in their intact molecular forms. Therefore the phase diagram of Hydrogen-Carbon-Nitrogen-Oxygen at high pressures and temperatures is of great interest. At moderate pressures (10s kbar), we computationally engineer new gas hydrates (H2O:N2, CO2, H2, CH4) and compute their stability ranges. Gas hydrates can form under moderate temperature and pressure conditions and as a result occur naturally on earth and within the solar system. They have applications in industry in

storage and transport of gases. This will be performed mostly using ab initio density functional theory techniques. At high pressures (100s GPa) the evolution of chemistry begins to dominate stability and novel compounds begin to appear. We can explore regions of this phase space using crystal structure prediction techniques.

Prediction of Rotational Raman Spectra for Hydrogen at High Pressure
Peter Cooke (Edinburgh)

At low temperature and pressure Hydrogen forms an HCP lattice of quantum rotors, known as Phase I. As pressure is increased to 110 GPa a phase transition is observed. The transition corresponds to a breaking of rotational symmetry of the rotors. However, Phase I covers a wide expanse of the phase diagram and it is not completely understood if free rotors persist in all regions. The nature of the rotors and excitations in each phase are typically deduced from Raman spectra, which are challenging to reproduce computationally. This means a comprehensive theoretical understanding has remained elusive. The model described here attempts to predict the rotational Raman spectra using a full quantum mechanical model of a set of rigid rotors. By comparing predicted spectra to experimental data we aim to further the understanding of Hydrogen under pressure and aid interpretation of experimental observations.

Quantum criticality near the Mott transition
Heike Eisenlohr (Technical University, Dresden)

The Mott metal-insulator transition is believed to be of first order, with the transition line terminating in a classical critical end point at finite temperature. Recent experiments in organic salts and numerical studies with dynamical mean-field theory have concordantly observed quantum critical scaling of the resistivity in the supercritical regime, which conventionally indicates a nearby quantum critical point at T=0. However, the studied system shows only a classical first order transition at T=0. So far no theoretical model was proposed to identify the degrees of freedom which behave as if they were quantum critical, and why. We propose to study the Hubbard hamiltonian as a paradigmatic model for strong correlations via dynamical mean-field theory, but in contrast to the previous works, use the numerical renormalization group (NRG) as an impurity solver. NRG implements scale separation, i.e. the successive elimination of high-energy modes, and is therefore suited to analyse critical behaviour.

Electronic Raman Spectrum of Twisted Bilayer Graphene
Aitor Garcia-Ruiz Fuentes (Bath)

Raman spectroscopy can be used to extract a wealth of information about graphene-related materials such as the number of layers, defect density, doping level or presence of strain in the sample. In all those cases, the Raman shift, equal to the difference between the energies of the incident and detected photons, arises because part of the energy is spent on exciting the crystal lattice of graphene. However, purely electronic processes in which the final state contains an electronic excitation, can also give rise to a Raman shift. It has been predicted and later confirmed experimentally that in monolayer graphene, a Raman process resulting in the creation of an electron-hole pair leads to a characteristic linear feature in the Raman spectrum, a consequence of the linear electronic density of states. Here, using the

continuum model for twisted bilayer graphene, we investigate theoretically the contribution of electronic excitations to its Raman spectrum. We present a description of electronic Raman scattering in graphene, as well as a continuum model for twisted bilayer graphene. We predict the presence of peaks in the spectrum induced by the interaction of the two layers, whose position and intensity are sensitively dependent on the twist angle.

Superconductivity Mediated By Strong Hubbard Repulsion
Manjinder Kainth (Birmingham)

We present a large U Hubbard model which explores the phase diagram of many unconventional superconductors; paramagnetism, ferromagnetism, anti-ferromagnetism, and superconductivity are observed.

A DFT+U study of the modulated antiferromagnet UAu2
Harry Keen (Edinburgh)

Abstract: TBA

First-principles Study of Complex Oxides
Can Kocer (Cambridge)

In this work, we study complex oxide materials from first principles. These materials are promising lithium-ion battery electrodes. Using density functional theory calculations, we can predict electrochemical profiles, phase evolution, and spectroscopic properties. By comparing our results to experiments, we gain insight into structure-property relationships and help design the next generation of energy storage materials.

Electronic properties of transition-metal dichalcodenides alloys
Siow Mean Loh (Warwick)

In this work, we utilize linear-scaling density functional theory (LS-DFT) to investigate the electronic properties of a transition-metal dichalcodenide alloy - Mo 1−x W x S 2 . We have used bandstructure projection techniques to calculate the effective bandstructures of disordered realisations of the cell at a range of concentrations. The results for the behaviour of the band gap, bandwidth and spin-orbit coupling agree well with recent ARPES measurements by our collaborators. We have also used a combination of STEM-ADF image analysis and Monte Carlo modelling of possible alloy configurations to determine whether these alloys are likely to display any short-ranged order. In the current material no deviation from perfect alloying can be observed.

Superconducting quantum circuits with Majorana fermions
Elena Lupo (Surrey)

The theory and the engineering of the Transmon qubit [1] was the first step toward the creation of a 2-level system which is suitable for the Quantum Computing and more robust that the previous Cooper Pair Box against some decoherence effects [2]. Recently, the study

of Topological states of matter and in particular Majorana Fermions in Topological 1D Superconductors has led to new ideas about the exploitation of these quasi-particles in hybrid Superconducting circuits devices [3, 4]. In this poster I present my first studies about the advantages of using these topological hybrid devices instead of the Transmon qubits, about the decoherence effects affecting them and about their possible gates operations.

Temperature dependence of magnetostriction: An ab initio theory
George Marchant (Warwick)

Magnetostriction, the spontaneous deformation of ferromagnets under the application of a magnetic field, has seen wide application for decades as a method for extracting mechanical work from magnetic energy. The sensitivity of a material's magnetostriction with respect to temperature is vital to its applicability. We therefore present a new, ab initio theory for calculating magnetostriction at finite temperatures through the use of fully relativistic disordered local moment (DLM)-DFT. We study bcc Fe and Fe_{1-x}Ga_x (Galfenol), the latter being notable as a relatively new, versatile material in magnetostrictive applications. Our results provide a qualitative theory for BCC Fe's anomalous magnetostrictive temperature dependence, as well as helping confirm the importance of short range order in explaining Galfenol's magnetostrictive enhancement properties.

Vortices in Four Spatial Dimensions
Ben McCanna (Birmingham)

Systems with four effective dimensions could be engineered using one or more "synthetic dimensions". The principle is to couple internal states, then view them as lattice sites along an extra dimension. This lets us increase a system's dimensionality and implement artificial gauge fields. Synthetic 2D lattices have been proposed and experimentally demonstrated in both ultracold atomic and photonic settings. However, most focus in four dimensions so far has been on non-interacting models. We go beyond this to investigate the properties of vortices in a hypothetical weakly-interacting 4D Bose gas.

An exact power series representation of the Baker-Campbell-Hausdorff formula
Jordan Moodie (Birmingham)

The Baker-Campbell-Hausdorff formula is well known and given by Z = log(e^X e^Y) = X + Y + 1/2 [X,Y] + 1/12 [X,[X,Y] + 1/12 [Y,[Y,X]] + ···, where the dots represent an increasingly complicated expression. Considering the symmetric form of this formula, namely S(A,B)=log(e^A e^(2B) e^A), we find an exact power series representation in the matrix B. We find closed form A-dependent coefficients in the form of hyperbolic functions for all orders of B. Each of these coefficients represent an infinite number of terms in the original expansion, making truncation of the series much more controllable for small B but arbitrary A.

Exactness of Bohr-Sommerfeld quantisation for two exactly soluble non-central potentials
David Perkins (Birmingham)

We demonstrate the integrability of the Hamilton-Jacobi equation for two non-central potentials in spherical polar coordinates, and present complete solutions for the classically

bound orbits. We then show that the semiclassical method of Bohr-Sommerfeld quantisation exactly reproduces the bound state spectra of the corresponding quantum mechanical Schrodinger equations. One of these potentials has previously been analysed in parabolic coordinates; the results for the other are, to the authors' best knowledge, original.

Understanding solitonic excitations in the charge density wave ordered ground state of the In/Si(111) nanowire array from phonon theory

Sammad Razzaq (MPI-Dusseldorf)

The Si(111)-(4x1)/(8x2)In atomic wire array is an extremely popular model system for one-dimensional electronic systems. It features a reversible temperature-induced metal-insulator transition into a charge density wave (CDW) ordered ground state. Solitonic excitations of the CDW and associated topological edge states are presently the focus of increasing attention. We carried out a combined *ab initio* and scanning tunneling microscopy (STM) study of solitonic phase defects in the In/Si(111) atomic wire array. We show how the solitonic CDW excitations can be modeled in terms of collective excitations of particular phonon modes. In conjunction with STM measurements, this phonon expansion approach allows us for the first time to determine the atomistic structure of the solitonic excitations. Due to the topological properties of the solitons and a strongly non-linear phonon-phonon coupling, these solitons interact in a deterministic way and are suitable for information processing. Financial support from the German Research Foundation (DFG), grant no. FOR1700 is gratefully acknowledged.

Implementing Superconductivity into a Green's Function (KKR) Method

Tom Saunderson (Bristol)

There is a plethora of problems regarding our understanding of the interaction between superconductivity and magnetism. One example is recent theoretical work on Sr2RuO4 [1] which is predicted to have cooper pairs with an intrinsic orbital magnetic moment. The focus of this work is on spin-dependent transport phenomena induced or influenced by the superconducting state as exemplified by the spin Hall effect [2]. Of crucial importance in the understanding of transport effects is the correct consideration of impurities and interfaces. In order to fully include all these aspects into the description of the electronic and magnetic properties of superconducting materials, we are implementing the Bogoliuobov-de Gennes equation into a Green's function (KKR) density functional theory method [3]. By using a Green's function method, it is possible to model problems containing impurities and interfaces without the need of supercells. This will provide insight into the coupling between superconductivity and magnetism influenced by impurities and ultimately spin-orbit coupling. Here we are going to present first steps in the implementation and discuss the challenges and advancement made so far.

DMRG studies of the Hofstadter model: Developing tools to classify topological phases on the cylinder

Leon Schoonderwoerd (Kent)

We develop tools to investigate Fractional Quantum Hall states and other topological phases in the Hofstadter model on an infinite cylinder geometry. These tools are built upon Matrix Product States and the Density Matrix Renormalization Group. We benchmark our methods on the $\nu = \frac{1}{3}$ Laughlin state. A main improvement over previous works is the calculation of entanglement entropy for various magnetic flux densities.

Weak Localization in Graphene with Strong Proximity Spin-Orbital Effects
Frederico Sousa (York)

The study of quantum corrections to the conductivity in graphene with proximity-induced spin-orbit interactions is a challenging task due to the complex interplay between pseudo-spin (sublattice) and real spin degrees of freedom. Recent studies1 focused on the effect of weak spin-orbit coupling (SOC) and Gaussian matrix disorder. In this work we present a theory of weak antilocalization (WAL) in graphene with large proximity-induced spin splitting due to interfacial breaking of inver-sion symmetry. We employ a self-consistent diagrammatic approach to sum the complete series of the maximally crossed diagrams, which allows us to access the regime of well-developed SOC with strong spin-sublattice mixing. Similarly to 2DEGs2, the spin relaxation lengths associated with dif- ferent Cooperon channels are found to be sensitive to the ratio of disorder broadening to SOC energy scales. These results are relevant for graphene-transition metal dichalcogenides 2D heterostructures displaying strong WAL magneto fingerprints3.

Incommensurate magnetism in UAu2 and development of a magnetic susceptometer for high pressure studies
Callum Stevens (Edinburgh)

Here we discuss experiments on the frustrated incommensurate antiferromagnetic (AFM) UAu2, showing non-Fermi liquid behaviour at low temperatures. Neutron diffraction measurements are presented on the magnetic structure of UAu2, compared to behaviour seen in heat capacity and resistivity measurements. The design and intended future measurements of an AC susceptometer for high pressure studies are discussed.

Quantum Monte Carlo study of biexcitons and trions in quantum rings
David Thomas (Lancaster)

Confinement of holes to quantum rings allows stable charge complexes such as trions and biexcitons to form [1,2]. Photons emitted from these complexes are regularly observed in photoluminescence experiments with quantum rings. In this work, quantum Monte Carlo methods [3] have been used to obtain highly accurate binding energies for these different complexes. This then allows the dependence of the binding energy on the exact size and or shape to be investigated. An effective mass approximation has been used to model the charge carriers, with the ring being modelled as an infinite confining potential for the holes. Trial wave functions describing this situation have been developed and subsequently optimised using the variational quantum Monte Carlo method. Binding energies for each complex are obtained from diffusion Monte Carlo calculations of the ground-state energies. All the complexes are found to be bound for experimentally relevant ring geometries [1], in agreement with observations of them, and with binding energies on the order of a few meV.

Long-lived non-equilibrium superconductivity in a non-centrosymmetric Rashba semiconductor
Philipp Verpoort (Cambridge)

Systems out of equilibrium can display exciting behaviour in disagreement with the laws of equilibrium thermodynamics. The dynamical processes in such systems crucially hinge on the existence of specific symmetries. Experiments have probed the magnetodynamics in the Rashba-superconductor GeTe, which lacks inversion symmetry in the bulk. It is found that at low temperature the system relaxes on time scales exceeding conventional electronic scattering times by many orders of magnitude. This reveals a non-equilibrium magnetoresponse that is asymmetric under magnetic field reversal and, strikingly, induces a non- equilibrium superconducting state distinct from the equilibrium one. We capture the qualitative features of the data and discuss the origin of the emergent long timescales based on the Rashba model. Our work provides novel insights into the dynamics of non-centrosymmetric superconductors and Rashba systems in general.

Path Integral Molecular Dynamics Simulations of Lennard-Jones Solids
Heather Wiebe (Edinburgh)

The Lennard-Jones (LJ) potential is one of the simplest and most popular models used to describe the interaction of neutral particles. Previous calculations have found the solid LJ system to have a hexagonal close packed (hcp) structure at low temperature, which transitions into a face-centered cubic (fcc) structure upon heating. However, these calculations were classical in nature and are thus only relevant to heavy noble gas solids. Application of this model to lighter gases such as hydrogen or helium necessitates a consideration of the quantum character of the nuclei. In this work, we use the Path Integral Molecular Dynamics (PIMD) technique to investigate the quantum effects on the relative stability of hcp and fcc LJ solids.

Transport of Bosons in One-Dimensional Channels
Rory Whelan (Birmingham)

One-dimensional quantum systems behave very differently to higher dimensional ones due to the enhanced effect of interactions and correlations between particles. One such system is a one-dimensional wire connecting two three-dimensional reservoirs of particles. Fermionic systems of this type are of interest due to their topological features, for potential uses in quantum computation. The equivalent bosonic systems are also interesting, with current discontinuously changing as a function of applied phase difference. This poster details how this current behaviour is found for a single channel system and how it can be generalised to a two channel system.

Nickel(II) cyanide as a physical realisation of the anisotropic
Emma Wolpert (Oxford)

One-dimensional statistical mechanical models continue to assume a particular importance in contemporary condensed-matter physics. Common themes amongst one-dimensional systems are (i) the absence of long-range order and (ii) the emergence of collective behaviour (e.g. in the form of quasiparticles with their own continuous excitation profile).

Much of the focus within the field thus far has been on systems with one-dimensional electronic or magnetic behaviour, yet, it has long been known that the one-dimensional Ising model is also relevant to the structural behaviour of some bulk phase. This mapping can be used to interpret otherwise unexpected physical properties of these fundamentally important systems. In our work we consider the problem of structural disorder in the layered inorganic material nickel(II) cyanide and demonstrate its relevance to a simple one-dimensional model of interacting anisotropic quaternions. The continuous degrees of freedom in the model are related to those of the S=1/2 particle. Our more general interest is in establishing meaningful correspondences between complex structural states and exotic magnetic and/or electronic phases in order to develop physical realisations of the latter for detailed study or exploitation.

Magnetism in Uranium Thin Films

Ming-Hung Wu (Bristol)

Uranium, a light actinide metal that has itinerant electrons in the 5f band, has been investigated in past decades for its complex properties. 1 It shows a large variety of different crystal structures such as α (orthorhombic), β (bct), γ (bcc) and hcp phase and its strong spin-orbital coupling makes Uranium a promising material for spintronics applications. 2 Especially in magnetic multilayer systems the proximity between a heavy, large spin-orbit coupling, material and a ferromagnetic material promises interesting new behavior. For this reason Uranium has been investigated in multilayer systems for 3d-5f hybridization with ferromagnet metals such as Fe, Co and Ni. 3-5 However, in order to understand the complex physics in multilayer systems, we first focus on the properties of the Uranium surface. From our ab initio calculations we predict magnetic moments on the surface of α, γ and hcp phases in stark contrast to their corresponding bulk phases. For bcc in (100) and (111) termination, the magnetic moments are almost entirely induced in the outermost layer and decrease dramatically going deeper into the thin film. In contrast, for hcp Uranium the magnetic moment persists only in the thinnest films, but vanishes in thicker systems, even for its surface layer. Monolayer α uranium becomes magnetic as well, which is in agreement with a published theoretical work.