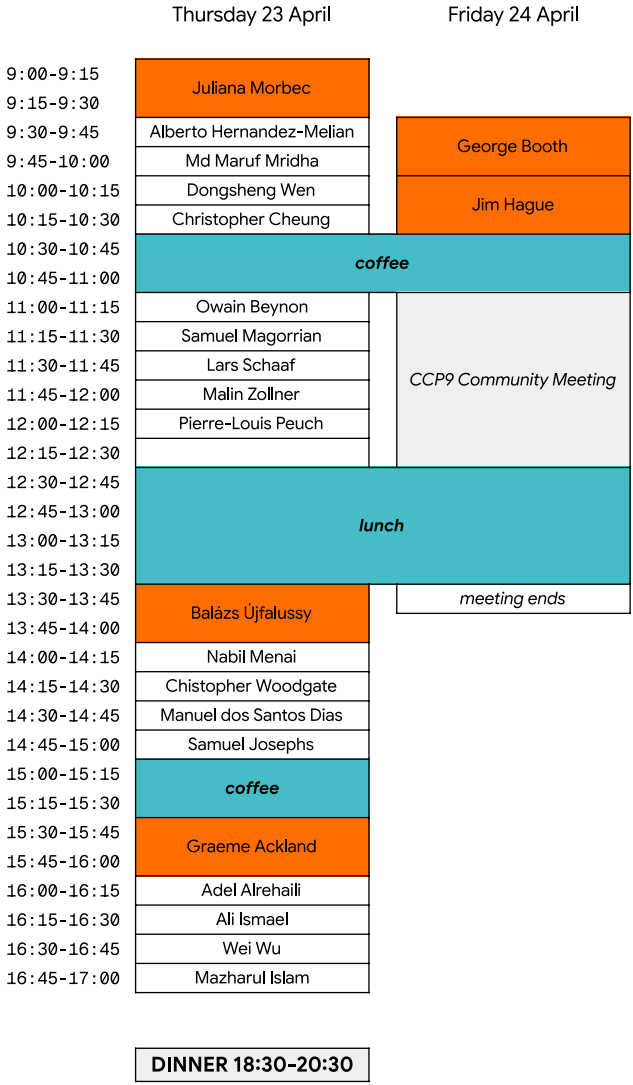
CCP9 Conference & Community Meeting

Delta Hotels Marriott, Liverpool, UK

21–24 April 2026

Programme and Abstracts

	Tuesday 21 April	Wednesday 22 April
9:00-9:15		Bo Peng
9:15-9:30		
9:30-9:45		Samuel Ladd
9:45-10:00		Ben Zelin
10:00-10:15		Oscar van Vuren
10:15-10:30		Gabriel Bramley
10:30-10:45		***coffee***
10:45-11:00		
11:00-11:15		Joseph Prentice
11:15-11:30		
11:30-11:45		Alistair Brewin
11:45-12:00		Miguel Luque Canete
12:00-12:15		Sunil Taper
12:15-12:30	*registration*	Chris-Kriton Skylaris
12:30-12:45	***lunch***	
12:45-13:00		
13:00-13:15		
13:15-13:30		
13:30-13:45	*Welcome: Stewart Clark*	Ivana Savic
13:45-14:00	Keynote: Arash Mostofi	
14:00-14:15		Aritra Roy
14:15-14:30		Amit Chaudhari
14:30-14:45	CONQUEST/David Bowler	Scott Habershon
14:45-15:00	ONETEP/Nick Hine	Visagan Ravindran
15:00-15:15	***coffee***	
15:15-15:30		
15:30-15:45	CASTEP/Stewart Clark	Luke Rhodes
15:45-16:00	CRYSTAL/Barry G Searle	
16:00-16:15	CASINO/Neil Drummond	Piotr Kowalski
16:15-16:30	QUESTAAL/Jerome Jackson	Hrishit Banerjee
16:30-16:45		Ty Mason
16:45-17:00		*IOP: Caroline Mitchell*
	POSTERS 17:00–19:00	**PANEL 17:30–18:30**


Thursday 23 April
Friday 24 April
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Juliana Morbec
Alberto Hernandez-Melian
Md Maruf Mridha
Dongsheng Wen
Christopher Cheung
coffee
Owain Beynon
Samuel Magorrian
Lars Schaaf
Malin Zollner
Pierre-Louis Peuch
lunch
Balázs Újfalussy
Nabil Menai
Chistopher Woodgate
Manuel dos Santos Dias
Samuel Josephs
coffee
Graeme Ackland
Adel Alrehaili
Ali Ismael
Wei Wu
Mazharul Islam
George Booth
Jim Hague
CCP9 Community Meeting
meeting ends
DINNER 18:30-20:30

Emergent behaviour of moiré transition metal dichalcogenides

Arash A. Mostofi *(Imperial College London)*

The superposition of two regular, but slightly different patterns results in a visually striking long-range interference effect known as a moiré pattern and, if you look closely, you will see examples of it in everyday life. Moiré patterns can also be created at the atomic scale by stacking and twisting 2D materials such as graphene and transition metal dichalcogenides. These moiré materials exhibit emergent and tunable electronic, vibrational and optical properties that are not possessed by their constituent layers. In this talk I will describe how we use a multi-scale theory and simulation approach to study the emergence of chiral phonons, surfing electrons, and optical excitations in moiré transition metal dichalcogenide bilayers and our strategies for overcoming the computational bottlenecks associated with dealing with moiré unit cells with thousands of atoms.

Recent Progress with CONQUEST: Large Scale DFT

David Bowler *(University College London)*

I will describe recent progress with the large scale and linear scaling DFT code CONQUEST, focussing on how DFT calculations on thousands of atoms are routinely available on relatively modest computing clusters.

Large-Scale DFT with ONETEP 8: New Capabilities and Applications

Nicholas Hine *(University of Warwick)*

The ONETEP Linear-Scaling DFT code has been the focus of extensive development effort over many years, most recently through the EPSRC-funded "Software For Research Communities" project, "Supporting research communities with large-scale DFT in the next decade and beyond". This developed new functionality, including a new GPU port, spin-dependent NGWFs, extended SOC capabilities and Brillouin zone sampling combined with hybrid delocalised/extended NGWFs. Recently this has been joined by new geometry optimisation capabilities, a new implementation of Real-Time TDDFT and a GPU port of the sparse matrix algebra library. In this talk I will discuss the impact of these new features for users, and demonstrate applications to topics such as electrochemical nucleation of gold on graphene, 2D material heterostructures, and catalytic transition metal oxide nanoparticles.

Molecular Quantum Materials from First Principles

Bo Peng *(University of Cambridge)*

Molecular building blocks provide a versatile platform for exploring the exotic quantum phases and complex many-body physics. Here we demonstrate a showcase system based on pure-carbon, defect-free, charge-neutral fullerene networks [1-4], which can be constructed from a molecular synthon with quantised spins due to symmetry [5]. We report a rich variety of condensed matter models that are challenging to realise, including (1) antiferromagnetic spin-1/2 chain in Janus fullerene nanoribbons [6,7], (2) ferromagnetic Haldane fullerene monolayers [8], and (3) altermagnetic Shastry-Sutherland fullerene networks that can be continuously tuned into a quantum spin liquid phase [9]. Our findings open new a frontier for exploring quantum phenomena based on scalable, chemically-stable, molecular building units can potentially operate at room temperature.

References:

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Strong and Weak Non-Adiabaticity in Equilibrium: Towards Exact Electron-Nuclear Correlation Beyond the Born—Oppenheimer Approximation

Samuel Ladd *(Durham University)*, S. Chavda, R. Sibley, N. Drummond and N. Gidopoulous

The Born–Oppenheimer approximation neglects non-adiabatic electron–nuclear coupling, limiting the accuracy of high-precision phonon and vibronic calculations and obscuring electron–nuclear coupling mechanisms beyond the adiabatic regime. We analyse equilibrium non-adiabatic phenomena as driven by a tension between minimising the electronic energy and minimising the mean curvature of the parametric electronic state over the nuclear configuration space. In model systems, we demonstrate that weak non-adiabaticity from nuclear zero-point motion can shift phonon and vibronic spectra relative to their adiabatic counterparts through phonon localisation. In a regime of strong non-adiabaticity, the exact electron–nuclear response induces topologically protected kinks in many-electron excited states, even where one might expect the adiabatic approximation to be accurate. We conclude with ongoing efforts to capture non-adiabatic phenomena in real systems.

New Atomistic Insights into Yield Anomalies in $L1_2$ Intermetallics

Benjamin Zelin *(University of Oxford)*

We investigate the long-standing question of why only some $L1_2$ intermetallics exhibit a positive temperature dependence of flow stress. While prior explanations have largely focused on differences in stacking fault energies, experimental measurements of these quantities are highly uncertain and scattered. Using density functional theory, we compute stacking fault energies and γ-surfaces for ten well-characterised $L1_2$ compounds spanning the full range of observed yield behaviour. By correlating atomistic fault energetics, fault stability, and elastic properties with experimental yield data, we show that several widely accepted yield-anomaly models are inconsistent with underlying atomistic trends. Instead, our results point to the superpartial dislocation core structure, particularly the role of complex intrinsic stacking faults, as a key factor governing anomalous yield behaviour.

Workflows for QM/MM Simulations of Metal Oxides

Oscar van Vuren *(Cardiff University)*

Multiscale QM/MM embedded cluster methods provide an attractive alternative to periodic DFT for materials simulation due to reductions in computational cost and inherent aperiodicity, eliminating finite cell errors in defect calculations. Despite this, QM/MM sees limited use due to the significant complexity involved in the construction of these models, requiring many parameters to be optimised. We have developed workflows to simplify and standardise the set-up of QM/MM models for use in the simulation of heterogeneous catalysis. By systematically evaluating the optimal QM region size and shape we can ensure that electronic and energetic properties of catalytic materials are captured accurately, following previous work in this field. These workflows have been effectively applied to ionic systems, giving accurate neutral and charged point defect formation energies in bulk MgO, as well as neutral defect formations and small molecule adsorptions on MgO surfaces. The transferability of the models produced using the workflow as evaluated by taking parameters derived from MgO and applying them to a ternary magnesium aluminium oxide spinel. The workflows are readily available in the ChemShell QM/MM software package, so that new users of QM/MM can quickly construct and use effective models for novel systems.

Implementing Extendable Workflows for QM-in-QM Embedding

Gabriel Bramley *(Cardiff University)*, Pavel Stishenko, Oscar van Vuren, and Andrew Logsdail

High-level quantum mechanical (QM) simulations provide accurate electronic information of chemical systems but scale unfavourably with system size. Hierarchical quantum mechanics in quantum mechanics embedding (QM-in-QM) addresses this issue by describing a small region of interest with high accuracy electronic structure methods and the wider environment with a less expensive embedding potential. However, implementing embedding procedures into established QM software packages can be challenging due to their monolithic design and complex software of many electronic structure packages. Our talk presents a modular and open-source approach that extends QM-in-QM embedding to electronic structure codes with reduced development overhead by using the Atomic Simulation Interface (ASI) application programming interface (API) to communicate data objects between QM code invocations. We demonstrate the new software, EmbASI, by implementing the projection-based embedding (PbE) scheme into the FHI-aims electronic structure software package. Furthermore, we show the significant compute time reductions enabled by QM-in-QM embedding for highly accurate post-Hartree Fock methods with negligible reductions in accuracy.

Understanding Environmental Effects on Crystalline Defects for Quantum Technology

Joseph C A Prentice *(University of Manchester)*, Henry Davis, James Bennett, Lucas Belz-Koeling, Kai Poh, Guangzhao Chen and Jason M Smith

Point defects in crystalline semiconductors are leading systems upon which many quantum technologies can be built, from quantum computing to sensing. However, fabrication processes such as ion implantation will necessarily lead to the presence of other defects, and experimental work has suggested that these can have a significant influence on properties. Here, we thoroughly examine from first principles how other defects can influence the properties of two significant colour centres in diamond - the N-V and Sn-V centres. We use several computational tools to characterise these systems: machine learning potentials to explore possible configurations, (linear-scaling) (time-dependent) density functional theory for electronic excitations and the coupling of vibrations to these excitations. We find that the influence of other defects can have a significant effect on observable quantities, and that this can explain experimental data. This suggests such effects must be carefully controlled when fabricating these systems for practical applications.

A Careful Analysis of Defect States in Cu_2O with DFT

Alistair Brewin *(Durham University)*, Stewart Clark and Matthew Jones

Cuprous oxide (Cu_2O) is of interest for several technologies, including solar cells, and more recently, quantum devices via Rydberg excitons. Its performance in these capacities is strongly affected by defects in the crystal. The current best diagnostic for the presence of defects in a sample is the photoluminescence (PL) spectrum, which shows a number of strong peaks at energies below the band gap, with brightnesses dependent on the sample. However, the assignment of PL peaks to particular defects has not been substantiated by modern theory. Using density functional theory (DFT), we investigate from first principles which native defects introduce electronic states within the Cu_2O band gap, and therefore would produce peaks in the PL spectrum. We find that the historic assignments of peaks to simple oxygen and copper vacancies are unsupported, and propose a new assignment based on oxygen and copper interstitials, and (one of the possible) split copper vacancies.

Phonon-Limited Conductivity of Topological Surface States in Bi_2Se_3

Miguel Luque Canete *(King's College London)* and Ivana Savic

Topological insulators, such as Bi_2Se_3, exhibit topological surface states (TSS) with promising applications where understanding their electronic transport properties is essential. At room temperature, electron-phonon interactions could significantly impact the conductivity of TSS, yet the dominant mechanisms of electron-phonon scattering remain unclear. In this work, we develop and validate a framework to compute the phonon-limited conductivity of the Bi_2Se_3 TSS using the Boltzmann transport equation in the relaxation time approximation. We include scattering with acoustic and non-polar optical phonons via deformation potential coupling. Acoustic phonons are obtained from the anisotropic elastic continuum equations and non-polar optical phonons from an extended slab model and density functional theory. In addition, we introduce an anisotropic dielectric continuum model to account for long-wavelength optical phonon scattering. All physical parameters entering the framework can be obtained from ab-initio calculations. Applying the framework to Bi_2Se_3 TSS, we quantify scattering rates arising from distinct phonon modes and evaluate their contributions to the temperature-dependent transport properties of TSS.

Role of Local Cation Environment on the Formation Energy of Oxygen Vacancies in Ferroelectric $Hf_{1-x}Zr_xO_2$

Sunil Taper *(King's College London)*, Bo Cai, Nives Strkalj, Bartomeu Monserrat and Giuliana Di Martino

Non-volatile memory devices have emerged as a promising platform to reduce the growing global energy demands of the ICT sector. Among the various phenomena available to build non-volatile memory devices from, devices based on ferroelectricity have emerged as front runners. The discovery of sub 10 nm ferroelectricity in Si doped hafnia (HfO_2), has led to an explosion of recent research. Oxygen defects play a critical role which is central in both the stabilisation and electrical performance of ferroelectric hafnia-zirconia thin films. Yet the interplay between oxygen vacancies and zirconium doping remains unclear. In this work, we employ Density Functional Theory to elucidate how local cation environments introduced by zirconium doping, together with vacancy charge states govern the oxygen vacancy landscape in ferroelectric hafnia-zirconia ($Hf_{1-x}Zr_xO_2$). We demonstrate that nearest-neighbour cation configurations critically influence vacancy formation, lowering the formation energy of oxygen vacancies in ferroelectric hafnia-zirconia relative to undoped hafnia. Neutral oxygen vacancies coordinated by four zirconium nearest-neighbours exhibit the lowest formation energies; bonding analysis reveals that vacancy creation removes a pre-existing anti-bonding state, stabilising the defect. Increasing zirconium content raises the density of such energetically favourable configurations without significantly altering individual formation energies. Upon the charge transition to positively charged state ($q = +2$) vacancy induced anti-bonding states shift above the Fermi level, further reducing the energetic cost of formation and increasing the number of accessible vacancy sites, suggesting that electric-field-induced charge transitions can facilitate vacancy diffusion. This work clarifies how doping and charge state modulate the defect landscape, offering a blueprint for tuning oxygen vacancy behaviour and, by extension, the performance of next-generation ferroelectric devices.

Linking Atomistic Simulations on Supercomputers to Larger Scales for Designing Better Batteries

Chris-Kriton Skylaris *(University of Southampton)*, Arihant Bhandari, Jacek Dziedzic, John Owen, Alberto Hernadez-Melian, Clare Grey, Robert Weatherup, Zac Goodwin and Denis Kramer

We are developing software for supercomputers for atomistic electrochemical simulations under operational conditions in order to capture the essential chemistry and physics of devices such as batteries but also provide the parameters needed for bridging atomistic with higher scale continuum simulations. Our developments are within the ONETEP program [1], which is based on a linear-scaling reformulation of density functional theory (DFT) that allows simulations of orders of magnitude more atoms than conventional DFT approaches, for more realistic models. In this talk, I will outline our developments, which include solvent and electrolyte models [2], and simulations at fixed voltage with respect to a computational reference electrode [3]. Also, I will describe our ongoing uses of the ONETEP linear-scaling framework combined with machine learning force fields to provide longer timescale simulations for processes such as the chemistry taking place during Solid-Electrolyte Interface (SEI) formation – a very complex multicomponent material crucial for battery operation. Finally, I will summarise recent applications of these tools to the process of lithium metal deposition on anodes and its competition with Li dendrite formation [4], one of the main mechanisms of battery degradation.

References:

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First-principles Based Model Approaches to Electron-Phonon Coupling in Semiconductors

Ivana Savic *(King's College London)*

The ability to compute electron-phonon coupling from first principles has enabled predictive calculations of electronic transport coefficients and ultrafast processes in crystalline materials. However, the state-of-the art first principles methods, which use density functional perturbation theory and interpolation techniques, are still computationally expensive. In this talk, I will present two inexpensive methods to obtain thermoelectric transport properties of semiconductors using a small number of electron-phonon matrix elements calculated from first principles. The first method combines models for coupling of electrons with different phonon modes whose parameters are obtained from first principles [1-3]. The second method uses machine learning to interpolate electron-phonon matrix elements [3]. I will illustrate the applications of these methods to calculate thermoelectric transport properties and ultrafast processes in bulk, 2D and topological materials [1-6].

References:

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ComProScanner: A Multi-Agent Based Agile Framework for High Quality Composition-Property Structured Data Extraction from Scientific Literature

Aritra Roy *(London South Bank University)*, Enrico Grisan, Chiara Gattinoni and John Buckeridge

In this presentation we will describe ComProScanner, an autonomous multi-agent platform that facilitates the extraction, validation, classification, and visualisation of machine-readable chemical compositions and properties, integrated with synthesis data directly from journal articles for comprehensive database creation using publishers' Text and Data Mining (TDM) API keys. We evaluated our framework using 100 journal articles against 10 different LLMs, including both open-source and proprietary models, to extract highly complex compositions associated with ceramic piezoelectric materials and corresponding piezoelectric strain coefficients (d33), motivated by the lack of a large dataset for such materials. DeepSeek-V3-0324 outperformed all models with a significant overall accuracy of 0.82. This framework provides a simple, user-friendly, readily-usable package for extracting highly complex experimental data buried in the literature to build machine learning or deep learning datasets.

Machine Learning Generalised DFT+U Projectors in a Numerical Atom-Centred Orbital Framework

Amit Chaudhari *(Cardiff University)*, Kushagra Agrawal and Andrew J. Logsdail

Accurate electronic structure simulations of strongly correlated metal oxides are crucial for the atomic level understanding of heterogeneous catalysts, batteries and photovoltaics, but remain challenging to perform in a computationally tractable manner. Hubbard corrected density functional theory (DFT+U) in a numerical atom-centred orbital framework has been shown to address this challenge but is susceptible to numerical instability when simulating common transition metal oxides (TMOs), e.g., TiO_2 and rare-earth metal oxides (REOs), e.g., CeO_2, necessitating the development of advanced DFT+U parameterisation strategies. In this work, the numerical instabilities of DFT+U are traced to the default atomic Hubbard projector, which we refine for Ti 3d orbitals in TiO_2 using Bayesian optimisation, with a cost function and constraints defined using symbolic regression (SR) and support vector machines, respectively. The optimised Ti 3d Hubbard projector enables the numerically stable simulation of electron polarons at intrinsic and extrinsic defects in both anatase and rutile TiO_2, with comparable accuracy to hybrid-DFT at several orders of magnitude lower computational cost. We extend the method by defining a general first-principles approach for optimising Hubbard projectors, based on reproducing orbital occupancies calculated using hybrid-DFT. Using a hierarchical SR-defined cost function that depends on DFT-predicted orbital occupancies, basis set parameters and atomic material descriptors, a generalised workflow for the one-shot computation of Hubbard U values and projectors is presented. The method transferability is shown for 10 prototypical TMOs and REOs, with demonstrable accuracy for unseen materials that extends to complex battery cathode materials like $LiCo_{1-x}Mg_xO_{2-x}$. The work highlights the integration of advanced machine learning algorithms to develop cost-effective and transferable workflows for DFT+U parameterisation, enabling more accurate and efficient simulations of strongly correlated metal oxides.

Physics-Informed Program Synthesis for Molecular Electronic Structure Calculations

R. Turanyi, K. Acheson and Scott Habershon *(University of Warwick)*

This talk will demonstrate a physics-informed program synthesis (PIPS) approach that can be used to identify new algorithms that accurately approximate the results of single-reference electronic structure approaches like Hartree-Fock (HF) and density-functional theory (DFT) - but without any self-consistent field iterations at all. Our PIPS strategy can be used to seek matrices M with eigenvectors corresponding to the same molecular orbital coefficients as converged HF or DFT calculations. We demonstrate this approach by generating new algorithms that accurately predict energies for heterodiatomic molecules (e.g. LiCl, LiF, NaCl, NaF) and C_1-C_4 hydrocarbons. Further simulations of C_8-C_{20} alkane species demonstrate further transferability and efficiency of the resulting algorithms. We obtain novel algorithms that can reproduce HF/DFT energies to within 0.1 kcal/-mol/atom - while requiring only a single matrix-diagonalisation operation.

Correlation Potentials in Solids from Inversion of Quantum Monte Carlo Densities

Visagan Ravindran *(Durham University)*, C. Johnson, N. D. Drummond, S. J. Clark and N. I. Gidopoulos

Over the last four decades, many density functional approximations (DFAs) have been proposed for the exchange-correlation (XC) energy and potential within Kohn-Sham density functional theory (KS-DFT). It has long been recognised that the accurate energetics from DFAs do not necessarily imply accurate KS potentials, i.e. functional derivatives of the total energy [1, 2]. The quality of the potential, in particular the XC potential, is however difficult to assess given it is not an observable. On the other hand, given accurate densities, one can "invert" the density to obtain accurate benchmarks of the exact XC potential, which has recently been applied to solids [3-5]. KS inversion alone however cannot separate the exchange and correlation contributions to the overall XC potential. In this work, we employ the inversion algorithm of Hollins et al. [3,6] to invert accurate QMC densities [4]. We then solve the optimised effective potential (OEP) equation to obtain the corresponding exact-exchange potential and hence benchmark exchange and correlation potentials for a range of insulating solids. We find that while the XC and exchange potentials are qualitatively similar, the correlation potentials are not. Moreover, we also compute the KS as well as generalised KS band structures in order to gauge the size of their derivative discontinuities.

References:

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Material-Specific Insights into Unconventional Superconductivity via Functional Renormalisation Group theory

Luke C. Rhodes *(University of St Andrews)*

Unconventional high-temperature superconductors, such as the cuprates, lanthanum nickelates, and iron-based superconductors, offer huge promise for future superconducting applications thanks to their transition temperatures above the boiling point of liquid nitrogen, high critical magnetic fields and possible potential for the development of qubits. However, this field has often been progressed by experimental trial and error, and predicting these properties in real materials from ab-initio has been a major challenge. Theoretical methods to describe the fundamental interactions behind unconventional superconductivity have been developed, using a technique known as functional renormalisation group theory (FRG), yet for decades this method have been so computationally demanding that it has only been applicable to the simplest of toy systems, limiting its utility for understanding real materials. A recent development, known as truncated unity functional renormalisation group theory (TUFRG), has however broken through this computation complexity barrier, enabling a route to connect the predicted correlated ground states, and transition temperatures, with material specific detail. In this talk I will discuss recent work we have been performing to apply this new technique to ab-initio electronic structures to both explain and predict the experimentally observed superconducting ground state and transition temperature of several real material systems. I will discuss the successes and limitations of this technique, as well as the opportunities it opens for future research and development.

Realistic Prediction of Electronic Structure of Materials for Energy Applications: Refining the DFT+U Approach

Piotr M. Kowalski *(Forschungszentrum Jülich)* and Kinga Warda

With the first European Exascale supercomputer installed at Forschungszentrum Jülich GmbH, advanced molecular-level simulations of electronic structures of large model systems are foreseen to drive designing of new, well performing and economically viable energy materials. In order to put simulation workflow on equal footing with experiment, the applied electronic structure methods must show accuracy exceeding that offered by standard density functional theory (DFT)-based approaches. We will discuss the enhanced performance of non-standard computational approaches such as the parameter free DFT+U method with Wannier functions-based projectors [1,2] or orbital resolved DFT+U approach [3,4] in describing d and f elements compounds. In particular, we identified severe overestimation of the occupancy of d and f orbitals by the widely applied DFT+U method as the origin of inaccurate prediction of electronic structure of various energy materials. This shortcoming is corrected by employing localised Wannier functions as projectors of orbitals occupancy [1,5]. Among others, this improvement revealed never considered before electronic structure of Fe-doped NiOOH, with Fe existing in the low-spin state at Fe contents below its solubility limit in NiOOH. The solution allows for consistent explanation of measured data on ionic and electronic structure, magnetic and electrochemical properties of this material [5,6], as well as wide range of other materials considered, for instance, for energy storage.

References:

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Applying Many-Body Physics Methods to Understand and Mitigate Degradation in Battery Cathode Materials

Hrishit Banerjee *(University of Dundee)*

In this talk, we examine the impact of degradation in commercially relevant Li-ion battery cathodes, and suggest mitigation strategies for such degradation. Taking the example of $LiNiO_2$ (LNO), a high-capacity cathode, which is prone to oxygen loss via the formation of singlet oxygen, we demonstrate spontaneous O_2 loss from the (012) surface of charged LNO, singlet oxygen forming in the process. We find that the origin of the instability lies in the pronounced oxidation of O during delithiation, i.e., O plays a central role in Ni-O redox in LNO. For $LiNiO_2$ and NiO_2 dynamical mean-field theory (DMFT) calculations yield a Ni charge state +2, with O varying between –1.5 (LNO) and –1 (NiO_2). Calculated XAS Ni K and O K-edge spectra based on GW Approximation (GWA) show excellent match with experimental XAS, confirming the predicted charge states. Singlet oxygen formation is caused by the singlet ground state of the peroxide ion, with preferential release of $1O_2$ rather than $3O_2$[1]. DMFT calculations on rhombohedral LNO show for the first time a gap of combined Mott and charge-transfer character and the ligand hole state. The paramagnetic insulating band gap is in excellent agreement with experiments and is in sharp contrast to DFT calculations[2]. We show that for NMC characterised by strong covalency between the transition metal and oxygen, DMFT calculations are essential to calculate charges and hence assign oxidation states accurately. Due to charge transfer from O p to Ni d, a ligand hole forms on O in Ni-rich regions. O has dual redox behaviour, showing greater involvement in redox in Ni-rich regions while showing negligible redox involvement in Ni-poor regions. The dual behaviour of O in terms of participation in the redox process helps explain the overall higher relative stability of lower Ni content NMCs compared to Ni-rich NMCs or LNO in terms of O loss and evolution of singlet oxygen[3]. The formation of Rock Salt Layer is also attributed to this O loss behaviour which hinders Li-transport[4] however we suggest an effective method of preventing such O loss by means of coating these cathodes[5]. Further we elucidate the redox mechanism in Li-rich high Ni-content materials and compare this to layered Ni-rich materials [6].

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Bridging Theory and Experiment with Dynamical Mean-Field Theory

Ty M. Mason *(University of Bristol)*, A. D. N. James and S. B. Dugdale

Density functional theory (DFT) is long established as a powerful technique for understanding and predicting the electronic structure of a diverse range of metals. Its reliability in metals is evidenced by the quantitative agreement of its predictions with a wide range of experimental probes, including Fermi surfaces from quantum oscillatory methods [1,2], and Compton Scattering [3,4], alongside other probes sensitive to the electronic structure [5]. Although incredibly powerful and successful, conventional DFT has can fall short when strong electronic correlations play a dominant role such as in the transition metal oxides and sulphides. Going beyond conventional DFT and combining it with DMFT (DFT+DMFT) has been shown to be a successful approach to reducing these discrepancies [6,7]. In my talk, I will discuss our implementation of DFT+DMFT in the Elk code [8] and show examples of its ability to improve agreement with experiment in materials such as NiO and NiS_2 [9].

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Defect Engineering in Monolayer Penta-$BeAs_2$ for Enhanced Gas Sensing

Juliana M. Morbec *(Keele University)*

Defects in two-dimensional materials can play a crucial role in modulating their electronic properties, which is particularly important for applications in gas sensing where sensitivity and selectivity are key. Monolayer penta-$BeAs_2$ has recently attracted attention due to its tunable electronic structure, high surface-to-volume ratio, and mechanical stability, making it a promising candidate for next-generation gas sensors. In this work, we employ density functional theory calculations to systematically investigate the effects of different intrinsic and extrinsic defects on the electronic and adsorption properties of monolayer penta-$BeAs_2$. We analyse how these defects alter the electronic density of states, charge distribution, and adsorption energies for common gas molecules, providing insight into defect engineering strategies to enhance gas sensing performance. Our results highlight the potential of defect modified penta-$BeAs_2$ as a tunable and efficient two-dimensional gas sensing platform.

Multiscale Battery Simulations: DFN Parameters and SEI Models from the Atomistic Level

Alberto Hernández-Melián *(University of Southampton)*, Arihant Bhandari, Jon Chapman, Colin Please, Andrea Giudici, Nicola Courtier, Denis Kramer, Erik Björklund, Conor M. E. Phelan, Jack E. N. Swallow, Zachary A. H. Goodwin, Robert S. Weatherup, Clare Grey and Chris-Kriton Skylaris

The atomistic simulation of battery materials provides a complementary, first-principles route to determine microscale properties which are needed for macroscale continuum models but sometimes difficult to extract experimentally. The ONETEP program [1] (onetep.org), developed for large-scale quantum atomistic calculations of complex systems, offers extensive capabilities for simulating battery materials in electrolytes and under applied voltage [2]. These capabilities also make it ideal for training machine-learning (ML) interatomic potentials [3], which deliver quantum-level accuracy at a fraction of the computational cost and thereby extend the scope of our battery simulations. Our current work follows two complementary directions. In collaboration with the developers of the PyBaMM library [4], we are creating a multiscale workflow that incorporates atomistically computed parameters (e.g. lithium diffusion coefficients) required by continuum models such as the DFN (Doyle-Fuller-Newman) battery model implemented in that library. Working with the Faraday Degradation Project, we are also building a digital model of the solid-electrolyte interphase (SEI) at the atomistic level. This model enables a deeper understanding of the reactions that govern SEI formation and evolution, with the goal of mitigating issues such as dendrite growth and electrolyte degradation that limit capacity and performance. Ultimately, these multiscale approaches where atomistic simulations inform battery behaviour at larger length scales will improve the predictive capability of continuum models and can be transferred to other energy-storage materials beyond lithium (e.g. Na-ion batteries, etc).

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Using Dynamics to Determine the Ground State Properties of g-C_3N_4

Md Maruf Mridha *(London South Bank University)*, Suela Kellici and John Buckeridge

Graphitic carbon nitride (g-C_3N_4) is a promising photocatalyst with unique structural, electronic and thermodynamic properties that at present requires a favourable semiconducting co-catalyst for efficient water splitting performance due to its poor charge mobility and fast photogenerated charge recombination. g-C_3N_4 may exist in three phases, but there are many outstanding questions regarding its ground state properties. Here, we perform a thorough investigation of the ground state structural and electronic properties of all three phases of g-C_3N_4, including bulk and single layer systems, using a range of density functional theory approaches. By investigating second order phase transitions, we determine the dynamically stable ground state configurations of each phase, finding that the system will "buckle" substantially even in the bulk phases, and that this buckling or corrugation occurs within moieties, not just among them. We find that the fundamental band gap varies by over 2 eV, depending on structure. Moreover, the bulk and surface energetics indicate that real samples may contain multiple phases and structures, and that the measured band gap is most likely an average value. We also compute band alignments with regards to the redox potential lines that vary strongly with structure and which indicate that preferential buckling may be beneficial for photocatalytic water splitting. Finally, analysis of the charge distributions of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) suggests that buckled structures may offer more favourable water oxidation and reduction sites, although for efficient activity co-catalysts will be required. Our study provides key information on this important material that may help the design of efficient photocatalysts for H_2 production.

Decoupling Structural and Electronic Dimensionality: 2D Transport in a 3D Honeycomb Chiral Stacking $HfSn_2$

Dongsheng Wen *(University of Liverpool)*, Hai Lin, Katie Scott, Jorge Cardenas-Gamboa, Iñigo Robredo, Batoul Almoussawi, Craig M. Robertson, Marco Zanella, Elisabetta Mariani, Aimo Winkelmann, Thomas Beesley, Luke M. Daniels, Michael W. Gaultois, Matthew S. Dyer, John B. Claridge, Maia G. Vergniory, Quinn D. Gibson, Claudia Felser, Matthew J. Rosseinsky and Jonathan Alaria

The widely accepted "structure-composition-function" materials design paradigm benefits from the control of the electronic structure followed that of the atomic orbital overlaps to access exotic functionalities. This straightforward coupling of the dimensionalities of the electronic structure and of the bonding makes complex our ability to combine the desired functionalities in low-dimensional electronic structures (for example, 2D transport in graphene) and 3D crystal structures (for example, chirality). In this study, we first theoretically demonstrated that quasi-2D electronic states can exist in 3D scaffolds with honeycomb stackings where orbital overlaps are equivalently strong in all directions. These states originate in the honeycomb layers that are present in $HfSn_2$ but hidden by the three-dimensional bonding. Chiral stacking of the honeycomb retains its electronic states in the presence of the strong interlayer orbital overlap. We then report the experimental observation of the 2D transport in the 3D $HfSn_2$ with chiral-stacked honeycomb layers, which is dominated by its 2D electronic component with nontrivial electronic topology, despite the strong 3D orbital overlap. This demonstrates that structural and electronic dimensionality can be decoupled by control of the arrangement of extended low-dimensional motifs to retain their electronic structures and augment functionality through the symmetry of the resulting scaffolds.

Charge-Transfer Induced Charge Density Waves in Twisted $NbSe_2/MoSe_2$ Bilayers

Christopher T. S. Cheung *(Imperial College London)*,
Arash A. Mostofi and Johannes Lischner

Twisted bilayers of transition metal dichalcogenide (TMD) monolayers have been shown to exhibit novel optical and structural properties. For instance, twisted bilayers of the semiconducting monolayers WS_2 and WSe_2 host interlayer charge-transfer excitons. However, the properties of twisted bilayers formed by stacking a metallic and a semiconducting monolayer have not been reported yet. Monolayer $NbSe_2$ is metallic and hosts different types of charge density waves (CDWs), in which the Nb atoms move away from their high-symmetry positions. Recently, using first-principles calculations, we predicted that different types of CDW can co-exist in twisted bilayer $NbSe_2$ [1]. In this work, we study the atomic structure and CDWs of twisted bilayer $NbSe_2/MoSe_2$ using large-scale density-functional theory calculations. We find that CDWs are induced in the $MoSe_2$ layer due to charge transfer. Furthermore, the amplitude of the CDWs is modulated on the length scale of the moiré unit cell due to the localisation of charge in specific regions. Our work demonstrates that novel structural properties emerge in moiré superlattices and enables the nanoscale manipulation of CDWs.

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Application of Machine Learning Interatomic Potentials for Ferroelectric Perovskites

Owain T. Beynon *(King's College London)* and Chiara Gattinoni

With the advancement of AI methods in science, there is a need to harness recent developments for studying ferroelectric perovskites–materials of technological importance due to their switchable polarisation. Applications include catalysis, electronics, and superconductors, where domain formation between polarised regions, observed experimentally, is of interest for novel computing architectures. While ab initio methods offer high accuracy, the computational cost limits large-scale simulations needed to explore mesoscale phenomena e.g. domains spanning hundreds of nanometres. Furthermore, the polarisability and changing valence states across phases hinder the development of reliable, low-cost classical force fields. AI-based approaches offer a solution through training machine learning models on quantum mechanical (QM) data. Machine learning interatomic potentials (MLIPs), trained on QM energies, forces, and structures, enable simulations with significantly reduced computational overhead while retaining QM-level accuracy. We present recent MLIP advancements applied to ferroelectric perovskites, facilitating the investigation of their electronic and structural properties.

Electronic Structure Considerations in the Training and Performance of Machine-Learned Force Fields

Samuel J. Magorrian *(STFC Hartree Centre)*, Ljiljana Stojanović, Lara Kabalan, Ardita Shkurti, Richard N. White, Fabian L. Thiemann and Viktor Zólyomi

Starting from MACE-UHTC [arXiv:2512.13204], a machine-learned interatomic potential model based on the MACE architecture and trained on low- and high-entropy mixtures of group 4 and 5 rocksalt transition metal carbides, we note a substantial difference in model performance between the group 4 and group 5 carbides. While the quality of energy and stress predictions is similar for all compounds, the quality of the model's force predictions deteriorates on going from group 4 carbides to group 5, especially for larger supercells. The additional valence electron in the case of the group 5 carbides gives a complex nested Fermi surface, with strong electron-phonon coupling and anomalous phonon spectra. We discuss the consequences of this for the training and performance of MLIP-derived force fields.

Towards Catalyst Design using Machine Learning Force Fields

Lars Schaaf *(University of Cambridge)*, Yicheng Wang, Fabian Berger, Angelos Michaelides, Charlie Sykes and Gabor Csanyi

Heterogeneous catalysis is central to modern industry and decarbonisation, but computational screening is often bottlenecked by the cost of evaluating many adsorption sites, intermediates, and transition states across realistic surfaces and coverages. In this talk, I will focus on using machine-learning force fields to evaluate barriers across entire reaction networks, enabling mechanistic screening beyond a handful of hand-picked steps. I will discuss the utility of foundation models as reusable starting points and how automated fine-tuning can adapt them to specific catalyst chemistries and operando environments with targeted high-level reference data. I will close with a brief outlook on developments that could further expand the scale and reliability of ML-enabled catalyst screening.

A 1,500-Molecule Multireference Benchmark for Excited States in Organic Semiconductors and Reliable Discovery of INVEST Emitters

Malin Zollner *(University of Strathclyde)*, Yashar Moshfeghi and Tahereh Nematiaram

Accurate prediction of excited-state energetics is essential for the rational design of organic semiconductors that enable next-generation optoelectronic technologies [1]. Yet widely used single-reference methods, most notably TD-DFT, can break down for precisely the systems of greatest chemical and technological interest. These include molecules with pronounced static correlation and those exhibiting inverted singlet–triplet gaps (INVEST) [2] a key target property for high-efficiency organic light emitting diode (OLED) emitters and emerging photovoltaic concepts [3]. We introduce the first multireference benchmark dataset tailored to small-molecule organic semiconductors. The collection comprises 1,500 chemically diverse π-conjugated compounds with systematically computed vertical excitation energies for S_1, S_2, T_1, and T_2, together with oscillator strengths for the lowest singlet transitions f1 and f2. All values are generated using a consistent multiconfigurational protocol based on state-averaged CASSCF and dynamical correlation via strongly contracted NEVPT2, providing a robust open-access reference for assessing excited-state methodologies on realistic materials motifs. Beyond the dataset itself, we perform a statistical interrogation of method-dependent errors to extract actionable guidance for practitioners. The analysis highlights when single-reference approaches remain dependable, when a multireference description becomes necessary, and which structural families are most susceptible to convergence failures or perturbative instabilities. Finally, we demonstrate how the benchmark enables materials discovery by screening for INVEST candidates relevant to OLED development. Strikingly, 126 INVEST molecules are identified only at the NEVPT2 level and are missed by TD-DFT and by CASSCF alone, showing that dynamical correlation is indispensable for reliable detection of technologically critical inverted-gap emitters.

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From Structure to Chemistry: Using DFT and Ionic-Radius Descriptors Enables Predictive Phase Mapping of Brownmillerite Oxides

Pierre-Louis Peuch *(Durham University)*, Emma McCabe and Nicholas Bristowe

Brownmillerites represent an highly adaptable family of oxygen-deficient perovskites, where the ordered vacancy network governs properties including ionic transport, magnetic response, and catalytic activity. However, predicting their adopted crystal symmetry remains challenging due to the presence of multiple competing phases with small energy differences between each other. Current phase maps depend on descriptors that can only be obtained after synthesis or extensive structural optimisation. By constructing a new phase map populated by first-principles density functional theory calculated ground states, we postulate a new predictive framework that removes dependence on structure-derived metrics. Further brownmillerite ground states are calculated using DFT to verify the self consistency and accuracy of this map. Our approach removes the need for any structure-derived metrics, offering a fast, chemistry-driven tool for pre-synthetic selection of the desired brownmillerite phase. This can guide the discovery of functional oxides for energy conversion, solid-state ionics, and strain-engineered applications, providing a clear path toward rational control of vacancy-ordered structures.

Superconducting Properties of Fe/Au/Nb Heterostructures form First Principles

Balázs Újfalussy *(Wigner Research Centre for Physics)*

In this talk, I generalise the fully relativistic screened Korringa-Kohn-Rostoker (SKKR) method for solving the corresponding Kohn-Sham-Dirac-Bogoliubov-de Gennes (KSDBdG) equations for surfaces and interfaces to describe their superconducting properties. As a first and most simple application we study the quasiparticle spectrum of Au overlayers on Nb host. We find that, within the superconducting gap region, the quasiparticle spectrum consists of Andreev bound states (ABS) with a dispersion which is closely connected to the underlying electronic structure of the overlayer. When combined with a semi-phenomenological parameterisation of the electron-phonon coupling a material specific model arises to calculate the superconducting critical temperature from the thickness dependence. In the case of Au/Nb heterostructures we obtain a very good agreement with experiments. Moreover, predictions can be made for similar heterostructures of other compounds. Extending our calculations to Fe covered Nb and Nb/Au multilayers, we show that the order parameters exhibit a Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) like oscillations in the iron layers, but more interestingly an oscillatory behaviour is observed in the gold layers as well. The band structure calculations suggest that this is the consequence of an interplay between the quantum-well states and ferromagnetism, and show a rather similar oscillatory behaviour of the critical temperature observed in experiments. Based on the calculations of the superconducting order parameter, the oscillatory behaviour observed in the experiments can be understood and calculated quite accurately at the same time. Similarly, experiments in epitaxial Nb/Au/Nb trilayers, the critical current density, the superconducting coherence length and the superconducting transition temperature all show an oscillating behaviour as a function of the Au-layer thickness. Such behaviour cannot be understood based on simple models of the Josephson effect. Using first principles theory, we study the effects of spin-orbit coupling, and the effect of confinement and show that they induce a complex structure of ABS which in turn modifies the quasi-particle spectrum and the Josephson supercurrent. Our study reveals the coexistence of two superconducting phases in the gold layers, the usual intraband s-wave phase and an additional FFLO phase stemming from interband pairing (without magnetic field). The results indicate the rich interplay between quantum size and proximity effects which suggests the possibility of modifying superconducting transport properties by exploiting thickness-dependent quantum size effects.

Large Intrinsic Spin Hall Effect Enabled by Spin-Orbit Coupling in the Altermagnet CrSb

Nabil Menai *(University of Bristol)*, Christopher D. Woodgate, Derek A. Stewart and Martin Gradhand

Altermagnetic CrSb combines compensated order with a large exchange-driven spin splitting near the Fermi level and a high Néel temperature, making it an attractive platform for spin-current generation. We compute the spin Hall conductivity (SHC) from first principles using Green's-function Kubo-Bastin transport. A coset decomposition of the nonrelativistic spin Laue group shows that the intrinsic SHC is symmetry-forbidden in the absence of spin-orbit coupling (SOC). When SOC is included, three symmetry-allowed SHC components emerge, reaching several hundred S/cm and displaying strong anisotropy, with magnitudes comparable to the prototypical antiferromagnet MnPt.

Spin Disorder and Electronic Correlations in Altermagnetic CrSb and MnTe Investigated Within the Disordered Local Moment Picture

Christopher D. Woodgate *(University of Bristol)*, Nabil Menai, Arthur Ernst, Julie B. Staunton

So called "altermagnets" are an intriguing class of magnetically ordered material in which there is a net zero magnetisation, but in which electronic bands are not spin-degenerate on account of the intrinsic symmetries of the underlying crystal structure. In the zero-temperature limit, the atomic magnetic moments (or "spins") will be arranged in a perfectly ordered, collinear structure. However, at any finite temperature, thermal fluctuations will cause the spins to deviate from this pristine arrangement. Above some critical temperature (the Néel temperature), long-range magnetic order disappears entirely, and the material transitions to a paramagnetic state. Here, we will present results of ab initio electronic structure calculations performed on two prototypical altermagnets: CrSb, which is metallic; and MnTe, which is semiconducting. We demonstrate that the magnetic phase transition in both materials is well-described by disordered local moment (DLM) theory [1-3] in combination with an appropriate choice of exchange-correlation functional, and describe in detail how site-diagonal spin disorder induces changes to calculated band structures. We provide preliminary estimates for the Néel temperature of both materials, and also discuss implications for temperature-dependent transport properties.

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Altermagnetic Magnons in CrSb from First Principles

Manuel dos Santos Dias *(STFC Daresbury Laboratory)*

Magnons are the elementary collective excitations of magnetic materials. They make a fundamental contribution to their quantum and thermal properties and can act as spin carriers for emergent magnonic devices. This motivates their systematic experimental investigation using inelastic neutron scattering and more recently resonant inelastic x-ray scattering (RIXS), and the development of theoretical methods for determining and understanding their behaviour. Magnons are typically obtained from linear spin wave theory based on a specified spin Hamiltonian, with the respective exchange interaction parameters determined either by fitting to experiment or by first-principles simulations for the material of interest. For the latter, applying the infinitesimal rotation approach using the Korringa-Kohn-Rostoker Green function (KKR-GF) method is quite natural and has proven very successful [1], for instance using the full-potential relativistic implementation developed in Jülich [2]. In this talk I will discuss CrSb, a metallic altermagnetic with the potential to also exhibit a strong altermagnetic splitting of its magnon spectrum, lifting the degeneracy expected for collinear antiferromagnets. Its magnon properties were investigated with RIXS and a strong circular dichroism was found at the magnon peak, while the conventional x-ray magnetic circular dichroism vanishes. This was explained by a minimal theory relating the x-ray photons to the spin excitations, and complemented with KKR-GF calculations for its magnetic exchange interactions [3].

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Automated Classification of Magnetic Skyrmions Without Machine Learning

Samuel Josephs *(Durham University)* and Stewart Clark

Magnetic skyrmions are topologically protected vortex-like spin textures characterised by a winding number[1] that have received significant attention due to their potential applications in memory devices[2]. Due to the long length scales involved the direct simulation of skyrmions via ab-initio methods such as density functional theory is intractable, however parameters for effective models such as the Heisenberg Model with the Dzyaloshinskii–Moriya interaction may be calculated[3,4,5]. These parameters may be used in a variety of effective models from which skyrmions may be obtained[6][7]. A key obstacle in the prediction of which materials may host skyrmions is the automated classification of these spin textures, with recent work making use of machine learning for this task[8][9]. I will review the physics of magnetic defects and relevant topology required to describe skyrmions, I will present a definition of a skyrmion in a multi skyrmion system beyond pure winding number considerations and a deterministic algorithm for their classification rooted in these concepts.

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Solubility in Metallic Hydrogen

Graeme J. Ackland *(University of Edinburgh)* and Jakkapat Seeyangnok Udomsilp Pinsook

The giant planets, Jupiter and Saturn, have vast magnetic fields which can only be due to metallic hydrogen layers. Conventional planetary models show layers of supercritical molecular hydrogen and metallic hydrogen, with He and Ne in the supercritical region. A core of rock and ice was proposed. The juno space mission attempted to study this core, and couldn't find it. We argue that this is because all elements, apart from He and Ne, dissolve in metallic hydrogen: the putative core would simply dissolve away. Solubility is a phenomenon little touched by electronic structure calculation, due to the central role of entropy which our field is reluctant to address. This is doubly problematic in complex fluids where regular solution models break down. We resort to large scale molecular dynamics calculation to shed some light on the problem. Such calculations require considerable care. If one simulates a single heavy atom in a sea of metallic hydrogen one calculates the binding energy of per atom, with noise proportional to the system size. Furthermore, hydrogen requires consideration of zero point energy. Nevertheless, we find that a wide range of elements (C, N, O, Be, B, S, Fe, Xe and La) are miscible in liquid metallic hydrogen. Even more remarkable are the "organic" elements C, N, and O. We find that these form well-defined molecular units. Compared with typical organic compounds, these "hypermolecules" are rich in hydrogen: CH_6, C_2H_{10} H_3O NH_4 CH_4OH. We interpret this as being that they are able to borrow electrons from the metal to form additional covalent bonds. We observe very long range charge oscillations around the hypermolecule, similar to the Friedel Oscillations of a charged defect in a free electron gas; whether this should be called an overall charge on the hypermolecule depends on the definition of which electron belongs to which atom. Plenty of other elements, and more complex hypermolecules remain to be investigated.

Single-Molecule and π-π-Stacked Dimer Electron Transport in Carbazole and Folded Bicarbazole Derivatives in Molecular Junctions

Adel Alrehaili *(Lancaster University)*, Ross J. Davidson, Juan Hurtado-Gallego, Asma Alajmi, Noorah Alwhaibi, Andrei Batsanov, Santiago Martin, Pilar Cea, Martin R. Bryce, Nicolás Agraït, Ali Ismael and Colin J. Lambert

The present work provides insight into how the conformations of flexible molecules can impact their single molecule conductance. Six thiol substituted carbazole-based molecules are synthesised and characterised. In four, two carbazole groups are joined by a linking group (1,3-propane or meta-xylene) while the remaining two are model mono-carbazoles. Using a combination of X-ray photoelectron spectroscopy (XPS), single molecule conductance measurements and density functional theory (DFT) calculations, we demonstrate that upon transitioning from a self-assembled monolayer (SAM) to a single-molecule junction the intermolecular interactions give way to intramolecular interactions. This resulted in the flexible bicarbazole molecular wires switching conductance mechanisms, which occurred primarily via the covalent conjugated aromatic part of the molecule in the SAM to one including conductance via non-covalent π-π interactions in the single-molecule junction.

Electronic Structure Investigation of Endohedral Metallofullerenes (EMFS)

A. Alajmi, B. Alanazi and Ali Ismael *(Lancaster University)*

For the purpose of creating single-molecule junctions, which can convert a temperature difference ΔT into a voltage ΔV via the Seebeck effect, it is of interest to screen molecules for their potential to deliver high values of the Seebeck coefficient $S = -\Delta V/\Delta T$. Here we demonstrate that insight into molecular-scale thermoelectricity can be obtained by examining the widths and extreme values of Seebeck histograms. Using a combination of experimental scanning-tunnelling-microscopy-based transport measurements and density-functional-theory-based transport calculations, we study the electrical conductance and Seebeck coefficient of three endohedral metallofullerenes (EMFs) $Sc_3N@C_{80}$, $Sc_3C_2@C_{80}$, and $Er_3N@C_{80}$, which based on their structures, are selected to exhibit different degrees of charge inhomogeneity and geometrical disorder within a junction. We demonstrate that standard deviations in the Seebeck coefficient σ_S of EMF-based junctions are correlated with the geometric quantity σ and the charge inhomogeneity σ_q. We benchmark these molecules against C_{60} and demonstrate that both σ_q, σ_S are the largest for $Sc_3C_2@C_{80}$, both are the smallest for C_{60} and for the other EMFs, they follow the order $Sc_3C_2@C_{80}$ >$Sc_3N@C_{80}$ > $Er_3N@C_{80}$ > C_{60}. A large value of σ_S is a sign that a molecule can exhibit a wide range of Seebeck coefficients and if orientations corresponding to high values can be selected and controlled, then the molecule has the potential to exhibit high-performance thermoelectricity. For the EMFs studied here, large values of σ_S are associated with distributions of Seebeck coefficients containing both positive and negative signs, which reveals that all these EMFs are bi-thermoelectric materials.

Functional Molecular Simulations

Wei Wu *(University College London)*

Molecular materials possess many excellent photomagnetic properties, making them suitable as carriers for numerous advanced functional devices. Here, we discuss research based on molecular materials in three areas: topological excitonology, light-driven spin-based quantum computing, and the adsorption of heavy metal ions. Our theoretical results, combined with relevant experiments, strongly demonstrate that the strong photoelectric response in molecular materials originates from the topological flat bands formed by molecular chains within molecular nanosheets. We also performed open quantum system simulations of spin-containing molecules. Finally, we combined advanced chemical synthesis characterisation with density functional theory calculations to explore molecular materials for heavy metal removal.

Thermodynamic and Electronic Properties of Wurtzite and Zincblende Based GaN Alloyed Compounds

Zijie Wang, Mazharul M. Islam *(University College London)* and David R. Bowler

Alloys of gallium nitride with aluminium and indium are gaining traction in optoelectronic applications due to their tunable direct band gap, which can theoretically span the full ultraviolet range — UV-A (315–400 nm), UV-B (280–315 nm), and UV-C (100–280 nm) — making them ideal for UV LEDs and photodetectors. In this study we provide a theoretical insight into the structural and thermodynamic stability, and electronic structure of alloy compounds with both perfect structure and near stacking faults. We carried out density functional theory (DFT) calculations to explore the relationship between structure and properties in $Al_xGa_{1-x}N$ and $In_xGa_{1-x}N$ alloys compared to pristine GaN, AlN, and InN. Our study suggests that there is less impact in thermodynamics, but pronounced impact on electronic properties for alloying in GaN. The calculated projected density of states (pDOS) reveals that the band gap has increased due to Al alloying whereas reduced due to In alloying compared to that in pristine GaN. The calculation of band densities shows that bands associated with the alloying element tend to localise around the stacking faults, with the In element showing more pronounced impact than Al. This indicates differences in band localisation among GaN, AlN, and InN, and gives insight into mechanisms that lie behind the segregation of alloying elements near stacking faults.

Coupling Quantum Algorithms to Classical Heuristics in Electronic Structure

George Booth *(King's College London)*

The NISQ era of quantum computing is limited to low circuit depths and uncorrected logical qubits. The question is then what we can do with them in the field of electronic structure, materials science and quantum chemistry. Describing quantum problems with quantum computers has long been touted as the 'killer app' of quantum computers, mainly due to the fact that the logical operations of quantum computers mirror those of Schrodinger equation in electronic structure. We take a critical look at this, and consider how to we can move beyond asymptotic scaling arguments and consider practical algorithms that leverage both classical heuristics and quantum enhancement to gain an advantage. In particular, we consider the 'variance problem' to extracting arbitrary observables from a quantum state, and how coupling the quantum problem to classical heuristics can improve this. While these approaches are expected to break down asymptotically, we find strong evidence that these large system arguments do not prevent algorithmic advantage from these simple protocols in many systems of interest. We further extend this to consider the extraction of beyond-energetic properties, as well as a natural combination within a quantum embedding framework. This avoids the unstable self-consistent requirements of previous quantum embedding approaches interfaced with quantum solvers, enabling application to realistic correlated materials science, where we demonstrate the volume-dependence of the spin gap of Nickel Oxide.

Reference: Lenihan et. al, ArXiv:2506.15438 (2025).

Quantum Simulation of Intermediate Correlation Materials

James Hague *(Open University)*

We calculate Hamiltonian parameters for cold (dressed Rydberg) atoms (DRAs) in arrays of optical tweezers and discuss how such arrays can be used to make quantum simulators for electron-phonon interaction and multi band effects in the presence of strong correlation. Arrays of optical tweezers are highly flexible: both depth and shape of individual lattice sites can be controlled dynamically for the quantum simulation of varied problems. Our goals are to understand how (1) quantum simulators can be used to emulate quantum materials in the weak- and intermediate-coupling regimes where multiple bands interact, and the basis is not localised and (2) Hubbard parameters differ between arrays of optical tweezers and standard optical lattices . We determine expressions for the hopping and Hubbard U of arrays of optical tweezers finding that strongly correlated systems with arbitrary structures can be simulated, including those with multiple-site basis and impurities [1]. We consider experimental parameters for quantum simulation of Hubbard models with an arbitrary basis. Finally, we discuss the onset of charge transfer insulating states in ionic Hubbard models. Finally, as proof of concept, density-functional calculations are made for the bandstructure for a 'graphene' quantum simulator made from arrays of optical tweezers [2]. We discuss our ambitions for design of quantum simulators using density functional approaches.

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Microscopic Mechanisms of Defect Dynamics in Ice Ih

Willem Farmilo *(University of Cambridge)*

As the most common form of ice in the biosphere, the I-hexagonal polymorph of ice has been the subject of considerable study for as long as we have been able to study it. In pure ice samples proton disorder persists following the Bernard-Fowler ice rules, which require first that there are two hydrogens bonded to each oxygen, and second that there is always one hydrogen occupying the site between every pair of oxygen atoms. These ice rules can be broken locally by what are known as ionic and Bjerrum defects. Ionic defects break the first rule by introducing an extra/missing proton in the form of an H_3O/OH species which can undergo structural diffusion at a rate observed to be orders of magnitude faster than in liquid water. Bjerrum defects, on the other hand, break the second rule by rotating of H_2O molecules to create empty/doubled hydrogen bonds (known as L/D defects). However, much remains unclear about the microscopic mechanisms of defect transfer, and a comprehensive study of temperature-dependent dynamics has yet to be completed, due to experimental/computational difficulty. This work aims to fill that gap using machine learning interatomic potential (MLIP) techniques in order to visualize defect dynamics in bulk ice Ih, with atomic resolution.

Tuning Macrocyclic Thermoelectrics via Thiophene Regioisomerism

Mona Alshammari *(Lancaster University)*, Asma Alajmi, Bashayr Alanazi, Alotaibi Hanadi, Adel Alrehaili, Alaa Al-Jobory, Colin Lambert and Ali Ismael

Quantum interference (QI) in single-molecule junctions exhibits robust effects at room temperature, which can be intuitively modelled using Quantum Circuit Rules (QCR) and Magic Ratio (MR) theory. These frameworks describe how molecular conductance is governed by constituent moieties and their connectivity. Here, we apply these principles to explore the thermoelectric properties of a series of macrocyclic structures featuring multiple electron pathways, with mixed meta and para connectivities. Our Density Functional Theory (DFT) calculations rationalise the experimentally measured conductance trends, demonstrating excellent agreement between theory and experiment. Furthermore, we predict that these macrocyclic junctions achieve significantly higher Seebeck coefficients than conventional single-branched analogues. A key finding is that strategic repositioning of sulfur atoms within the thiophene rings provides fine tuning of QI, modulating conductance by over two orders of magnitude. This structural tuning strategy constitutes a crucial design principle for multi-pathway molecular systems, as it enables precise electronic control without altering the fundamental quantum interference nature. Our work establishes macrocyclic architectures with tunable connectivities as a highly promising platform for advanced molecular thermoelectrics.

Development of High Specific Modulus Multicomponent Alloys with An FCC Structure

Mustafa Zahid Seker *(University of Sheffield)*, Colin Freeman and Russell Goodall

This project aims to design a new single-phase FCC High Entropy Alloy (HEA) with a high specific modulus, employing a combined computational and experimental approach. The goal is to develop a lightweight engineering material that achieves ductility through an FCC structure, and a high stiffness and low density, using the compositional freedom of HEAs. Firstly, computational modelling methods are used to efficiently explore the vast compositional space and identify promising candidates. After promising compositions are found through modelling studies, these alloys are manufactured experimentally, and the modelling results are verified by characterisation studies. In this direction, CASTEP, an atomistic modelling method based on density functional theory, is used in assessing lowest energy phases and their elastic properties. In addition to this method, phase estimation is supported using Thermo-Calc (CALPHAD method software). In the experimental side, Vacuum Arc Melting is used in sample manufacturing. SEM, EDX and XRD are used to characterise the structure, with mechanical properties assessed by nanoindentation.

Theoretical Characterisation of the Wurtzite and Zincblende GaN Stacking Faults

Zijie Wang *(University College London)*, Mazharul M. Islam and David R. Bowler

GaN crystallizes in two phases: the hexagonal wurtzite (wz) structure (most stable) and cubic zincblende (zb) structure (metastable phase). Both the wz and zb GaN epitaxial layers contain many planar defects, i.e. stacking faults (SFs). Here we have performed density functional theory (DFT) calculations to understand the structure, energetics and electronic properties of stacking fault defects. The most common basal SFs occurring in (0001) planes are three types of intrinsic (I1, I2 and I3) as well as one type of extrinsic (E). The zb GaN on the other hand consists of three types of SFs namely intrinsic, extrinsic and twin. We have studied the convergence of the formation energy with number of layers along the z direction in all these SFs. Based on the calculated formation energy, I1 is the most stable SF of wz GaN in accordance with the experimental observation. For the zb GaN, all three types of SFs have similar formation energy indicating that all three types are possible. The calculation of band densities reveals that near the Fermi level in wz GaN, the valence bands are localised below the boundary of the stacking faults, while the conduction bands are localised on the other side of the SFs. We observe the opposite behaviour in zb GaN, and present plots of the potential in the stacking fault cell relative to bulk to understand this behaviour. We have studied the band edges within the SFs, and find that they all behave similar to a type II QW (though the wz SFs are very sensitive to structural details). In the next step, we aim to understand the segregation of alloying elements in extended defects as well as study the defects with increasing dimensionality (1-, 2- and 3-D).

Real-Time TDDFT Investigation of Field-Induced X-ray Absorption in Copper Complexes

Shazma Gilani *(University of Lincoln)*, Joshua D Elliott and Matt Watkins

Ultrafast X-ray spectroscopies provide a direct probe of electronic motion in transition-metal systems, revealing how charge and orbital dynamics evolve on femtosecond timescales [1]. Capturing these processes theoretically remains challenging because conventional frequency-domain TDDFT often fails to reproduce field-driven non-equilibrium effects [2]. In this work, we employ real-time time-dependent density-functional theory (RTP-TDDFT), as implemented in CP2K, to simulate the Cu K- and L-edge absorption spectra of hydrated and ligand-coordinated Cu(I/II) complexes. A Gaussian-profile electric field is applied to mimic pump–probe excitation, and the time-dependent dipole moments are propagated for up to 300 000 steps (0.000046 fs time step). Fourier transformation of the dipole response yields XAS spectra whose edge positions and oscillator strengths vary systematically with field intensity and pulse duration. The results reveal transient redistribution of Cu 3d–ligand π^* character and a measurable shift ($\approx$ 1–2 eV) in the pre-edge feature, indicating strong coupling between the localised core states and photo-induced charge density. These findings demonstrate how RTP-TDDFT can directly connect external-field dynamics to experimentally observable X-ray spectra, offering a computational pathway toward interpreting ultrafast XAS of molecular catalysts and photoactive metal complexes.

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Impact of Cs_2CO_3 as Surface Modifier on ZnO in Hybrid Organic Light-Emitting Diodes: A Density Functional Theory Study

Rozy Hooda *(University of Chester)*, Jakub Korejwo, Theodoros A. Papadopoulos, Hong Li and Jean-Luc Bredas

Cs_2CO_3 has been widely used as an interlayer material in organic light-emitting diodes. Here, we report the results of a theoretical investigation, based on density functional theory calculations, of the Cs_2CO_3/ZnO interface of relevance to inverted device architectures. We explore the characteristics of a Cs_2CO_3 monolayer deposited on the ZnO surface in terms of: (i) adsorption geometry; (ii) electronic structure of the Cs_2CO_3/ZnO interface; and (iii) work-function modification of the ZnO surface. The results of our calculations indicate that charge transfer from the Cs_2CO_3 molecular layer to the ZnO substrate represents the leading contribution to the substantial work-function decrease of the ZnO substrate.

Artificial Dielectric Breakdown in Short Ranged Machine Learned Interatomic Potentials.

Isaac J. Parker *(University of Cambridge)*, Mandy J. Hoffmann, William J. Baldwin, Shuang Han, Srishti Gupta, Kara D. Fong, Angelos Michaelides, Christoph Schran, Sandip De and Gábor Csányi

Machine learned interatomic potentials (MLIPs) have enabled atomistic simulations with ab initio accuracy for a fraction of the computational cost. However, many widely used MLIPs are short-ranged and do not accurately capture long-range electrostatic interactions. In polar interfacial systems, such as those involving water, this deficiency can drive unphysical long-distance dipolar alignment far away from interface. Here we quantify how such dipolar alignment impacts the solvent electronic structure and show that spontaneous, artificial fluctuations of the total solvent dipole induce spurious metallization—a phenomenon we term "artificial dielectric breakdown". This breakdown is eliminated by MLIPs that explicitly include long-ranged electrostatics. Our results expose a generic failure mode of short-ranged MLIPs and establish long-range electrostatics as essential for obtaining accurate dynamical electronic properties from MLIP enhanced atomistic simulations of systems with a polar-liquid component.

Defining the Hubbard Manifold: Accurate DFT+U Method for d- and f-Electron Materials

Kinga Warda *(Forschungszentrum Jülich)* and Piotr M. Kowalski

Density functional theory (DFT) with Hubbard corrections is widely used for computation of materials with partially filled d and f shells, yet its accuracy depends critically on how the Hubbard manifold and projector functions are defined. In this work, we present a systematic assessment of orbital-resolved DFT+U (OR-DFT+U) [1] and Wannier function (WF)-based DFT+U schemes, employing Hubbard U values computed from the linear response method. Accurate modelling of lanthanide oxides is particularly challenging due to the highly localised Ln-4f electrons and their hybridization with Ln-5d and O-2p states. Here, we define the correlated subspace via maximally localised WF, which adapt to the local chemical environment enabling to capture metal-ligand hybridization [2]. This framework reproduces the band gaps of lanthanide sesquioxides (Ln_2O_3, Ln = La-Lu) and CeO_2 with deviations < 0.4 eV, and XPS spectra with high fidelity, outperforming conventional atomic-orbital projectors and achieving accuracy comparable to GW and hybrid functional calculations. For mixed d and f elements compounds such as ternary monouranates (AUO_4, A = Mn, Co, Ni), lattice geometries are strongly influenced by the interplay of localised U-5f and transition-metal 3d electrons with O-2p orbitals. Standard shell-averaged DFT+U tends to artificially over-localize these electrons, suppressing hybridization and yielding unrealistically high-symmetry structures [3]. By using OR-DFT+U, where the Hubbard manifold is restricted to the most localised A-3d, U-5f and O-2p orbitals, while excluding strongly hybridized states, we accurately capture structural distortions such as octahedral tilts [4]. This approach reproduces experimental lattice geometries with accuracy comparable to the DFT+U(WF) scheme. These findings demonstrate that accurate definition of the correlated subspace-whether via orbital resolution or Wannier projectors-is essential for reliable predictions of both electronic and structural properties in strongly correlated d-f materials.

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Universal Transport at Lifshitz Metal-Insulator Transitions in Two Dimensions

Harry Tomlins *(King's College London)* and Jan M. Tomczak

We study the charge transport across a band-tuned metal-insulator transition in two dimensions. For high temperatures T and chemical potentials μ far from the transition point, conduction is ballistic and the resistance $R(T)$ verifies a simple one-parameter scaling relation. Here, we explore the limits of this semiclassical behaviour and study the quantum regime beyond, where scaling breaks down. We analytically evaluate the simplest Feynman diagram of the linear-response conductivity $\sigma = 1/R$ of a parabolic band endowed with a finite lifetime. Our formula shows excellent agreement for experiments for a field-tuned $MoTe_2/WSe_2$ moiré bilayer, and can capture the quantum effects responsible for breaking the one-parameter scaling. We go on to discuss a fascinating prediction of our model: The resistance at the quantum-critical band-tuned Lifshitz point ($\mu = T = 0$) has the universal value, $RL = 2\pi h/e^2$, per degree of freedom, in congruence with experiment. Furthermore, we investigate whether two-dimensional metal-insulator transitions driven by strong electron correlations or disorder can also be classified by their quantum-critical resistance and come up with an, in principle, complete assignment of the transition mechanism.

Ionic Gating of a Meta-Connected Molecular Junction Achieves a 10^5 ON/OFF Ratio

Faizah Almutairi *(Lancaster University)*, Asma Alajmi, Colin Lambert, Ali Ismael

Tuning Quantum Interference Through Molecular Junctions formed from cross-linked OPE-3 dimers

Asma Alajmi, Adel Alrehaili, Mohammed Alzanbaqi, Karimah Alresheedi, Hanadi Alotaibi *(Lancaster University)*, Ali Ismael and Colin Lambert

This poster highlights a novel strategy for tuning the electrical conductance of single molecules by cross linking the molecules to form a dimer. We demonstrate that the appearance of destructive or constructive quantum interference in cross-linked OPE-based dimers is independent of the nature of the molecular cross link. Instead, the type of the interference is controlled by the connectivity to external electrodes and is determined by the presence or otherwise of meta-connected phenyl rings in the transport path. This opens the way to a novel strategy for memristive switching.

Tuning Quantum Interference of the Ferrocene Unit

Karimah Alresheedi *(Lancaster University)*, Asma Alajmi, Adel Alrehaili, Kholood Alharbi, Mohammed Alzanbaqi, Hanadi Alotibi, Ali Ismael and Colin Lambert

We study four molecules to explore the effect of structural configuration and π-conjugation length on their electronic properties. Molecules 1 and 2 differ in the spatial arrangement of thiomethyl-substituted benzene rings—either on opposite sides (molecule 1) or within the same Cp ring plane (molecule 2), forming a conjugated system. Molecules 3 and 4 share similar arrangements, but with extended π-conjugated backbones due to the incorporation of ethynyl (alkyne) linkers. This design allows for a comparative analysis of how conjugation and molecular length influence electronic behaviour. Additionally, we examine how the conductance of molecules 1 and 3 change when the top ring is rotated relative to the lower ring. Remarkably, their rotation angle dependence changes when triple bonds are present in the linker groups connecting the core to the electrodes.

High Thermopower of Monolayers and Bilayers of C_{60} Derivatives

Mohammed Alzanbaqi *(Lancaster University)*, Bashayr Alanazi, Asma Alajmi, Colin Lambert and Ali Ismael

We use density functional theory to study the thermoelectric properties of a gold-molecule-graphene molecular junction formed a fullerene monomer (denoted PTEG-1), comprising a fullerene derivative with a polar triethylene glycol (TEG) pendent group and found that the Seebeck coefficient is +261 mV/K . This high positive value for the Seebeck coefficient is marked contrast with the high negative Seebeck coefficient of a gold-dimer-graphene molecular junction containing two anti-aligned PTEG-1 molecules which we found to be 356 mV/K . We also computed the Seebeck coefficient of molecule comprising C_{60} derivative attached to two ethylene glycol chains (denoted PTEG-2) in the presence of n-DMBI+ doping, which we found to vary between 109 mV/K and 205 mV/K , depending on the level of doping. These high values of the Seebeck coefficients with both positive and negative signs suggest that such molecules are ideal candidates for producing scalable gold-molecule-graphene thermoelectric generators.

Large-Scale First-Principles Modelling of Facet-Resolved Charging and Electrolyte Decomposition Kinetics at Lithium Metal Nanoparticle Interfaces

Brad Ayers *(University Of Southampton)*, Gilberto Teobaldi and Chris-Kriton Skylaris

Lithium metal anodes offer unparalleled theoretical capacity, yet their practical deployment remains limited by dendrite growth and the formation of a compositionally heterogeneous solid electrolyte interphase (SEI). In our recent work [1], we showed that applied voltage simultaneously governs lithium nanoparticle morphology and the binding preferences of SEI precursors, with carbonate consistently dominating over fluoride at the reducing potentials relevant to lithium deposition. That study, however, treated adsorption thermodynamics on periodic slabs and left open two important questions. First, how does charging distribute across the individual crystallographic facets of a realistic nanoparticle, rather than a single infinite surface? Second, does kinetic accessibility, rather than thermodynamic preference alone, ultimately control which decomposition products form the nascent SEI? We address both questions here through two complementary first-principles studies. In the first, we use the linear-scaling DFT code ONETEP [2] to simulate lithium nanoparticles exceeding 1500 atoms, constructed from the voltage-dependent Wulff shapes derived in our earlier work and embedded in implicit solvent and electrolyte [3] under grand canonical electrochemical bias [4]. For the first time, this allows us to resolve how charge accumulates differently on thermodynamically dominant facets such as 110 and 320, at the boundaries where facets meet, and at under-coordinated edge and corner sites. In the second study, we turn to the kinetics of electrolyte breakdown. Using Quantum ESPRESSO [5] with the Environ implicit solvation module [6], we compute activation energy barriers for EC and PF_6^- decomposition on the lowest-energy lithium facets via the nudged elastic band method [7]. Taken together, these two studies move our voltage-as-selector framework beyond idealised slab thermodynamics towards kinetically informed predictions on realistic, multi-faceted nanoparticle models of the lithium-electrolyte interface.

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Accelerating Superconductivity Searches in Ternary Hydrides

Maélie Caussé, Kieran Bozier *(University of Cambridge)*, Peter I. C. Cooke, Stefano Racioppi and Chris J. Pickard

The high-pressure hydrides are among the most promising candidates for high temperature superconductivity. Following the successful discovery of many superconducting binary hydrides, attention has shifted to the vast chemical space of ternary hydrides, resulting in discoveries such as $LaSc_2H_{24}$ [1] and Mg_2IrH_6 [2]. However, screening through these ternary systems presents a major challenge, due to the expanded composition space required to evaluate thermodynamic stability, combined with the high computational cost of electron-phonon density functional perturbation theory (DFPT). In this work, we address this challenge by employing machine-learned potentials designed to accelerate structure searching and the construction of the ternary convex hull. Trained on small but diverse unit cells, these potentials enable random structure searching orders of magnitude faster than standard DFT. We identify numerous dynamically stable and thermodynamically metastable candidates with high predicted critical temperatures, including $YSbH_6$ with a T_c of 120 K [3]. Finally, we also discuss new techniques to accelerate and enhance the accuracy of superconducting property calculations.

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First-Principles Phonon Screening of Excitons in III-V Semiconductor Materials

William Bunting *(University of Oxford)*

Search for Superconducting Ternary Hydrides at Moderate and Low Pressures with EDDPs

Maélie Caussé *(University of Cambridge)*, Kieran Bozier, Peter Cooke, Stefano Racioppi and Chris Pickard

Computational methods have revolutionised material discovery, driving interest in designing new advanced materials, e.g., superconductors, which exhibit zero resistivity below a critical temperature (T_c). Reaching pressures in the 100 GPa range enables the synthesis of superhydrides, a new class of hydrogen-rich materials that exhibit remarkable properties such as superconductivity, hydrogen diffusion, and hydrogen storage. A striking example is LaH_{10}, which holds the record for the highest superconducting transition temperature at $T_c = 250$ K [1,2], and showcases high hydrogen diffusion at high temperatures [3]. However, stabilising such compounds at ambient or low pressure remains a major challenge for practical applications. This has driven the search beyond binary hydrides toward ternary superhydrides, aiming to discover new superconductors with high critical temperatures that can persist near ambient pressure. The discovery of new superconducting hydrides traditionally relies on ab initio crystal structure prediction and experimental synthesis. However, ab initio calculations become computationally prohibitive, e.g. for assessing the thermodynamic stability of complex systems such as ternary superhydrides, due to the extremely vast chemical space. To overcome this limitation, our group has successfully developed tailored machine learning interatomic potentials – ephemeral data-driven potentials (EDDPs) – enabling a great acceleration in structure prediction [4]. This approach was used to build the convex-hull of a new predicted metastable ambient-pressure hydrogen-based superconductor Mg_2IrH_6 with a T_c of 160 K [5]. I will highlight how EDDPs revolutionise our high-throughput search workflow, and showcase our recent prediction of a new ternary hydride superconductor [6].

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Tight-Binding Modelling for the Phonon-Guided Generation of Hot Carriers

Damian Contant *(King's College London)*, Leonardo Biancorosso, Johannes Lischner and Ivana Savić

In the field of photocatalysis, metallic nanoparticles (NPs) stand as ideal candidates to induce chemical reactions in molecular adsorbates [1]. A direct illumination at specific frequencies generates plasmons on the NP surface. Their decay can then lead to the formation of hot electrons and/or hot holes under the Landau damping process, which, when transferred to the adsorbates, modifies the activation profiles [2,3]. Another non-radiative decay pathway involves the vibrational excitation of the NP phonon modes. While this process is usually perceived as a cause of energy loss, it can also lead to a vibrational transfer to the adsorbate, thus potentially opening different reaction routes. To model these phonon-guided processes, we need to describe electron-phonon interactions within the metallic NPs. In this work, we seek to perform a tight-binding parametrization of the electronic band structure for systems featuring small atomic displacements away from equilibrium, in order to obtain a description of electron-phonon coupling [4]. We will present the fitting of the Slater-Koster parameters to density functional theory calculations for non-ideal bulk structures such as strained crystals, and the validation of whether such Hamiltonians can accurately describe electron-phonon coupling.

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First-Principles Phase Behaviour of Nanoconfined Water at Extreme Conditions

Ioachim Dusa *(University of Cambridge)* and Christoph Schran

Water confined at the nanoscale is vital in geology, biology and materials science. It influences biological processes, clay behaviour and catalysis. Compared to bulk water, nanoconfined water displays markedly different properties, including enhanced diffusion and altered phase behaviour, making it both scientifically and technologically important. Its electronic structure, conductivity, viscosity, and phase transitions govern its behaviour in energy storage, CO_2 capture, and nanofluidic systems. However, simulating confined water at first-principles accuracy is computationally expensive, with traditional density functional theory limiting molecular dynamics to picosecond timescales. Recent advances in machine learning potentials - such as MACE and Allegro - enable nanosecond-scale simulations at ab initio accuracy. While confined water already exhibits exotic phases with unconventional structural and transport properties at moderate pressures and temperatures, access to more extreme thermodynamic regimes is required to reveal additional structural complexity and to investigate the onset of electronic phase transitions.

Low Energy Effective Theory and Magnetic Excitations in a Star-Lattice Antiferromagnet

Marios Georgiou *(University of Leeds)*

Dimethylammonium copper sulfate $[(CH_3)_2(NH_2)]_3[Cu_3^{II}(\mu_3\text{-}OH)(\mu_3\text{-}SO_4)(\mu_3\text{-}SO_4)_3]\cdot 0.24H_2$, DiMACuS for short, is the first material realising a spin-1/2 star-lattice antiferromagnet [1]. Recent experiments [2] report anisotropic magnetic responses and a 1/3 magnetisation plateau for fields applied along the crystallographic c-axis, suggesting the presence of anisotropic interactions beyond simple Heisenberg exchange. A minimal model derived from density-functional theory, consisting of inequivalent exchange couplings on weakly coupled triangular units together with a sizable Dzyaloshinskii–Moriya interaction explains the experimental magnetisation data. Building on this model, we determine the ground state configuration and compute the excitation spectrum as well as the dynamical structure factor using the multiboson method, providing insight into the collective magnetic excitations and the underlying physics of this frustrated star-lattice magnet [3].

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Developing Dynamical Mean-Field Methods for Actinide Materials Simulation at AWE

Sean Harding *(AWE)*

Electronic structure simulations for actinide materials are complicated by the propensity of the 5f electrons to form strongly correlated ground states. To capture these states for accurate materials simulation, a combination of efficient density functional theory (DFT) and many-body methods, chiefly Dynamical Mean-Field Theory (DMFT) is required. Several questions of industrial importance require models which describe the influence of a local perturbation on the electronic structure. Examples include describing the surface chemistry of a solid, or structural relaxations in the bulk due to a defect. To simulate such effects in conjunction with strong correlations requires scalable and accurate DMFT implementations that can work with large unit cells, even when neglecting nonlocal correlations. Ongoing work to develop such a capability at AWE is presented.

Large Scale Simulations of Hydrogen Diffusion in Plutonium Oxide

Stuart Hope *(University of Southampton)*, Ben Ellis, Philip Keenan and Chris-Kriton Skylaris

Plutonium oxide is an critical material for nuclear energy. It is a highly toxic material capable of self-ignition, and susceptible to structural erosion during long-term storage. The primary mechanism of structural change is self-irradiation. Alpha decay events generate high-energy recoil atoms that displace surrounding lattice atoms, producing a cascade of defects. While approximately 90% of these atoms will return to their lattice positions, thousands of Frenkel pairs remain. Defected regions weaken structural stability and change the permeability of the material to small atoms like hydrogen, which can be spontaneously generated in storage, and subsequently diffuse through the material. With an estimated 30 of these events per million atoms per year, large-scale simulations are required, on the order of thousands of atoms, to reasonably simulate these events, under realistic conditions. [1] To achieve this we will employ linear scaling Density Function Theory (DFT), using the ONETEP code, [2] for high accuracy force and energy calculations. This work builds on previous defect studies carried out by our research group. [3] This code is used to find transition states and train machine learned inter-atomic potentials. This data can be used to simulate damage caused over long time spans and obtain diffusion coefficients over long timescales without requiring Molecular Dynamics (MD) simulations. This approach enables the prediction of long-term changes to the crystal structure and transport properties, primarily, diffusion coefficients. This will contribute to safer storage strategies and more reliable estimates of material lifetimes.

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Investigation of Piezo- and Ferroelectric Catalysts Using Atomistic Methods

Britanny M. Klassen-González *(King's College London)* and Chiara Gattinoni

Hydrogen has attracted an increasing amount of interest in recent years as a renewable fuel option. One of the most popular methodologies to obtain it is via photocatalysis, although the band gap and electron-hole recombination time in materials like TiO_2 reduces its feasibility. This has led to the search for other mechanisms enhanced by intrinsic properties, such as piezo- and ferroelectricity in ceramic perovskites. Combining the piezoelectric effect with catalysis, a new type of mechanism ensures water splitting: piezocatalysis. Barium titanate ($BaTiO_3$, BTO) is one of the most extensively studied materials among ceramic perovskites, presenting both piezo- and ferroelectricity, hence its importance and use in understanding piezocatalysis. Experimentally it has been shown to produce up to 300 µmol/gh with pure water and close to 900 µmol/gh with methanol as a sacrificial agent; in both cases, BTO nanocrystals between 50 and 100 nm were used (J.-D. Ai et al., 2023, 10.1002/cctc.202201316). Employing Density Functional Theory (DFT), we have studied the relation between tensile and compressive strain, and how these affect polarity in BTO slabs. The slabs are studied in a paraelectric and ferroelectric state, allowing us to understand the role that piezo- and ferroelectricity have in hydrogen production. Water splitting appears to present an increased activity in ferroelectric state with a-2% strain in the TiO_2 termination of the slabs, with a reduction in the bandgap from 0.38 eV to 0.25 eV.

Hubbard Interactions and Chirality Induced Spin Selectivity in Helical Molecules

Aadi Konidena *(King's College London)* and Lev Kantorovich

Chirality induced spin selectivity is an exciting phenomenon where the geometry of helicoid molecules evidently determines the resulting electron spin when a current is driven through the molecule[1]. Despite experimental backing, the details of the primary mechanism that drives spin selection is still not understood. In fact, theoretical simulations based on spin-orbit coupling alone still disagree substantially with experimental data, prompting the investigation into alternate rationales for the observed spin-polarised current. To assess the possible role of the electron-electron correlation effects in spin current polarisation, we study the quantum transport through a molecular junction with Hubbard interactions added on each site of a single-helix alongside the spin-orbit coupling. We employ the Non-Equilibrium Green's Function (NEGF) formalism and Feynman diagram technique to explicitly account for Hubbard interactions within the Second Born approximation. We iteratively solve the Dyson and Keldysh equations and self-consistently calculate the retarded and lesser Green's functions. Then we calculate the spin current as a function of the temperature and the applied bias, going beyond the simple Landauer approach into the Meir-Wingreen regieme.

A Density Functional Theory Investigation of Cs_2CO_3-Induced Work-Function Tuning of TiO_2 for Inverted Hybrid OLEDs

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Cs_2CO_3 is widely used as an electron-injection interlayer in organic light-emitting diodes. In this study a density functional theory investigation of Cs_2CO_3/TiO_2 interface, relevant to inverted device architectures is presented. A model of Cs_2CO_3 monolayer adsorbed on a TiO_2 surface is produced and examined with the preferred adsorption geometry, the interfacial electronic structure, and the resulting modification of the TiO_2 work-function being presented. This study is intended to clarify the mechanisms, such as possible interfacial dipole formation and charge redistribution, by which Cs_2CO_3 may tune the surface electronic properties of TiO_2.

Computational Modelling of Substituted Bullvalene Networks

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Bullvalene (BV) is a small, ten-carbon molecule in which strain-promoted Cope rearrangements lead to simultaneous breakage and reformation of carbon-carbon bonds, giving access to nearly 1.2 million degenerate isomers [1]. Upon substitution of the BV core, its isomers lose degeneracy and groups initially bound to neighbouring carbon atoms can end up on the opposite ends of the molecule through a series of Cope rearrangement giving various molecular shapes, dipole moments and stereochemistry at one point in time[2]. Owing to these unique properties, BV has been explored for guest [3] and metal-binding [4], host-guest chemistry [5], and as part of molecular glasses [6] and polymers [7]. Highly substituted BVs can have large equilibrium reaction networks of thousands non-degenerate isomers interconverting with each other and computational studies became crucial for supporting interpretation of experimental observations. [8,9] This poster discusses different isomer distributions in the networks of thiophene and thiophene oxide BV with 2100 non-degenerate isomers. The two networks can be interconverted via reduction/oxidation of the thiophene substituent becoming the first example of a switchable BV network of that size. Global network analysis of all shapeshifting and conformational isomers and transition states of the thiophene and thiophene oxide BV was achieved using in-house-developed bullviso code [10] and density functional theory (DFT) calculations. Kinetic analysis of 3125 reversible Cope rearrangements using Stochastic Monte Carlo simulations allowed to determine the most probable rearrangement pathways between the isomers and study evolution of the network over time. The computational results are in good agreement with NMR data.

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Simulating Oxygen Adsorption and Dissociation onto Platinum Electrocatalysts for PEM Hydrogen Fuel Cells

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With the recent push towards environmental sustainability and net zero targets, Proton Exchange Membrane Fuel Cells (PEMFCs) present a viable and versatile technology for both stationary and mobile energy source and storage applications. Currently, state-of-the-art PEMFCs use Pt-based electrodes to catalyse the Oxygen Reduction Reaction (ORR) which, while performant, have some key shortcomings. The ORR that occurs on the catalyst surface shows significant kinetic barriers that could be further reduced, while the electrocatalyst itself is both expensive, due to its precious metal composition, and susceptible to degradation. Thus, it is critical to understand how the morphology of the electrocatalyst and chemical environment of the catalytic reaction affect the efficiency of ORR and to understand the conditions in which degradation of catalyst by oxidation occurs; factors that can be hard to elucidate from experiment alone. In this project we perform large-scale Density Functional Theory (DFT) atomistic simulations[1,2] to study each step of the ORR reaction pathways independently. Here we focus on the adsorption of a single oxygen atom and O_2 molecule dissociation on both Pt surfaces and ideal nanoparticles on all symmetrically irreducible sites; investigating how the chemical environment affects the adsorption energies and reaction pathways when compared to in vacuum. We achieve this by applying an implicit solvent-electrolyte model [3,4] parameterised to fit operating conditions. For our future work, we aim to create more realistic simulations an operating electrocatalyst by exploring how the reactivity of the catalyst is affected by a solvent in conjunction with an applied external potential through grand canonical DFT simulations [5].

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Structural and Electronic Properties of Hafnia (HfO_2)

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Symmetry-Enabled Altermagnetism in the Hybrid Improper Ferroelectric $Ca_3Mn_2O_7$

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Altermagnetism (AM) has recently been identified as a distinct form of magnetic order in which time-reversal symmetry is broken in the absence of net magnetisation, resulting in spin-dependent band splittings that vary across momentum space and are enforced by crystal symmetry [1, 2]. This unconventional combination of spin-polarised electronic structure and fully compensated magnetic order enables magnetic functionality without the stray-field constraints associated with conventional ferromagnets [1]. These properties motivate interest in AM for spin-based technologies targeting low-energy operation, high integration density, and fast dynamics [3]. Beyond applications, AM has prompted a reevaluation of how magnetic phases are classified through the lens of spin-group symmetry [1, 2]. However, identifying the microscopic mechanisms that stabilise AM order in practice, as well as the parameters by which it may be tuned in real materials, remains a central open challenge [2]. In this work, we investigate the layered Ruddlesden–Popper oxide $Ca_3Mn_2O_7$ as a model system for exploring symmetry-enabled AM behaviour from a lattice-dynamical perspective. $Ca_3Mn_2O_7$ is a prototypical hybrid improper ferroelectric, in which a polar ground state arises from the condensation of two non-polar octahedral distortion modes relative to a high-symmetry parent structure, with the spontaneous polarisation induced by a trilinear coupling between these modes [4]. While the structural and magnetic properties of $Ca_3Mn_2O_7$ have been extensively characterised, these studies predate modern symmetry-based classifications of AM and therefore did not examine spin-dependent electronic structure within this framework [4, 5]. Recent work has further identified $Ca_3Mn_2O_7$ as a candidate AM multiferroic and reported non-relativistic AM spin splitting in its electronic structure [6]. Using DFT+U calculations in CASTEP combined with phonon analysis and symmetry-adapted distortion-mode decomposition, we examine how distortion-driven symmetry lowering modifies the magnetic symmetry environment [4].

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Synthetic-Data-Driven CNN for Robust Single-Atom Detection in Electron Microscopy Images

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Accurate detection of single atoms in noisy Scanning Electron Transmission Microscope (STEM) images is essential for characterizing single-atom catalysts. However, manual annotation is too slow for large-scale studies, and traditional automated tools often require excessive fine-tuning to remain reliable. We present a fully synthetic training pipeline for a compact Convolutional Neural Network (CNN) thatlocalizes single atoms. An Image simulator generates 128×128 px STEM-like images with 20–50 atoms ($\approx 8\%$ empty), smooth background blobs, and realistic noise. A 3-layer CNN trained with weighted binary cross-entropy and a phased-weight schedule (w_{pos}: $120 \rightarrow 1$) achieves high detection accuracy on a held-out test set. Per-image median normalization and local-maxima post-processing yield robust binary peak maps. The modular Prediction Model is readily transferable to experimental STEM data and forms the basis for high-throughput statistical analysis. Validation on experimental Pt/ C STEM image confirms the framework's robust performance in detecting single atoms.

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