MATERIALS AND MOLECULAR MODELLING HUB

and

The UK Car-Parrinello HEC Consortium (UKCP)

Conference & User Meeting 2025

Programme & Abstracts

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	Machine Learning for Spectroscopy of 2D Materials
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	Update from the Materials Theory Group
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	Multiscale Modelling: An Industrial Perspective
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	Machine Learning Interatomic Potentials: MACE Foundation Models and Electrostatics: Update from the Gábor Csányi group and University of Cambridge
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	Linking atomistic simulations on supercomputers to larger scales for designing better batteries
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15:20 – 15:40	**Samira Anker, University of Sheffield**
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	Sensible Asymmetric Units for Crystal Exploration
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	Molecular quantum materials from first principles
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15:30 – 16:15	**Andrew Morris, University of Birmingham** Strong electron correlations in Novel Battery materials
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Abstracts – UKCP

Phonons and their interactions in complex systems

Bartomeu Monserrat - University of Cambridge

Phonons and their interactions play a key role in many material properties, from their heat capacity to their conductivity. In this talk, I will introduce two software packages that we are developing to study phonons and related properties.

The first is Caesar, a finite difference phonon code that provides order-of-magnitude speed-ups compared to existing finite difference phonon codes. I will illustrate its capabilities by showing the calculation of phonons using dynamical mean-field theory as the underlying electronic structure solver in materials ranging from high pressure hydrides to nickelates.

The second is DaoQuantum, an electron-phonon and phonon-phonon code using linear response to evaluate phonon-driven quantities such as electron transport. I will illustrate its capabilities by showing the calculation of electron-phonon scattering in the presence of phonon dephasing, a contribution that we find to dramatically affect the electronic conductivity of metals.

I will also give a short overview of other projects supported by UKCP, including charge density waves in Kagome metals, topological excitons, and circularly polarised emission in organic systems.

Machine-learned interatomic potentials for mainstream materials modelling

Volker Deringer – University of Oxford

I will discuss recent advances in machine-learned interatomic potentials (MLIPs) for materials modelling, and in particular ongoing efforts on making MLIPs "mainstream" tools – accessible to a wide community of researchers and routinely enabling scientific studies, in the same way that direct quantum-mechanically based simulations have been for many years. This presentation will include an update on recent work carried out as part of our UKCP membership and discuss future perspectives.

Machine Learning for Spectroscopy of 2D Materials

Nicholas Hine, University of Warwick

Machine-learned models of the potential energy surface and of dielectric properties can reproduce the accuracy of density functional theory (DFT) while enabling dynamical simulations at significantly larger length and time scales with minimal computational cost. We present their applications to complex two-dimensional transition metal dichalcogenide (TMD) systems, including alloys and twisted bilayers, using machine-learned interatomic potentials (MLIPs). For alloys, we previously developed MLIPs for quaternary TMD systems of the form Mo1−xWxS2−2ySe2y, capable of predicting first-order Raman spectra, while for twisted bilayers, we introduced an MLIP for all like-chalcogen combinations of MoS2, WS2, MoSe2, and WSe2, capable of characterizing domain reconstruction at low twist angles. We now further expand our ML framework to predict dielectric properties, which, when combined with MLIPs, enables vibrational spectra calculations beyond the harmonic approximation. We apply this to alloys and aligned bilayers, demonstrating strong agreement with experimental spectroscopy data.

Materials Discovery with Ephemeral Data Derived Potentials

Peter Cooke, University of Cambridge

The development of Machine Learned Interatomic Potentials (MLIPs) has revolutionised atomistic simulations over recent years. MLIPs enable simulations with accuracy comparable to quantum mechanical approaches at up to 10 million times smaller computational cost. The ephemeral data derived potentials (EDDPs [1,2]) are a flexible class of MLIP that can utilise comparatively small neural networks for fast and accurate simulations. Materials discovery techniques, such as random structure searching, can exploit this acceleration in a number of ways. Larger system sizes and chemical spaces can be explored, or more computationally intensive structure optimisers, utilising molecular dynamics, can incorporated [3]. Through a range of applications, we demonstrate that more complex optimisers can improve search performance for large systems. Through example simulations in LAMMPS [4], we further show that the EDDPs can be employed beyond structure searching, to explore complex dynamical behaviour across a range of conditions and chemical systems.

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[2] P. T. Salzbrenner, S. H. Joo, L. J. Conway, P. I. C. Cooke, B. Zhu, M. P. Matraszek, W. C. Witt, C. J. Pickard, Developments and further applications of ephemeral data derived potentials, J. Chem. Phys. 159, 144801 (2023)
[3] C. J. Pickard, Beyond theory-driven discovery: introducing hot random search and datum-derived structures, Faraday Discuss., 256, 61-84, (2025)
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Multiscale Modelling: An Industrial Perspective

Misbah Sarwar, Johnson Matthey

Computational techniques to model material properties and catalytic behaviour have now become mainstream tools in an industrial setting. This is due to two main factors: improved algorithms that accurately model material behaviour and increased computational power enabling faster simulations. As such, multi-scale simulations, ranging from electronic structure to continuum-based approaches have become embedded in product development cycles, innovating the way in which new products are developed.

The talk will give an overview of how multi-scale modelling combined with advanced characterization techniques are being used in industry to understand the structure and activity of catalytic materials that are used to accelerate the transition to net zero. Multi-scale modelling aims to tackle the “grand challenge” of simulating catalytic processes by bridging atomic, molecular, pore, and reactor scales. However, it brings substantial challenges due to the complexity and diversity of phenomena involved, combined by the difficulties in aligning differences in temporal and spatial scales and handling the computational demands across each model layer. Using methane oxidation as a test case a multiscale workflow developed as part of the EU funded ReaxPro project will be presented. The developed models were validated against experimental data collected through different reactive characterisation techniques. Model predictions demonstrated reasonable agreement with experimental results without any experimental fitting of parameters, highlighting the workflow's potential for tackling the complexities inherent to industrial catalytic processes.

The talk will also discuss how newly developed approaches such as MLIPs might fit into such a workflow and be used to accelerate the catalyst discovery process.

Machine Learning Interatomic Potentials: MACE Foundation Models and Electrostatics: Update from the Gábor Csányi group and University of Cambridge

William Baldwin, University of Cambridge

MLIPs are rapidly becoming a standard tool used by computational chemists and materials scientists. Over the last few years, the technology of building MLIPs has evolved extremely rapidly. Where 4 years ago it would take months to build a model for simulating a single, relatively simple system, many architectures today can be used out of the box to generate highly accurate models with little difficulty. MACE is a key component of this body of work, being one of the most widely used (and therefore benchmarked) state of the art architectures. Our group is now addressing two new frontiers for MLIPs. Firstly, the construction of foundation models which are trained on huge databases covering the whole periodic table and which are able to simulate complex systems without additional user training. Secondly, the development of new architectures which incorporate electrostatic interactions.

This talk will first review the some of the current applications of MACE our group is pursuing, highlighting developments in software such as an efficient CPU implementation of MACE. Then I will discuss the current state of Foundation models, including the discussion of the most recent models and the importance of data quality, as well as extensive benchmarking tools we are developing. Finally, we will examine the progress towards general electrostatic models, considering our current guiding examples: metal-water interfaces and charged defects in semiconductors.

Linking atomistic simulations on supercomputers to larger scales for designing better batteries

Chris Skylaris, University of Southampton

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 development of new DFTB approaches within the ONETEP linear-scaling framework, which combined with machine learning force fields, provide longer timescale simulations for processes such as the chemistry taking place during SEI formation. 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.

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[2] Practical Approach to Large-Scale Electronic Structure Calculations in Electrolyte Solutions via Continuum-Embedded Linear-Scaling Density Functional Theory. J. Dziedzic, A. Bhandari, L. Anton, C. Peng, J. C. Womack, M. Famili, D. Kramer, and C.-K. Skylaris. J. Phys. Chem. C. 124 (2020) 7860-7872.

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Invited & Contributed Talks – MMM Hub

Hybrid QM/MM and Machine Learning for Zeolite Catalysts and Silica Polymorphism

Jamal Abdul Nasir, University College London

Jamal Abdul Nasir*, Alexey A. Sokol, Scott Woodley, Jingcheng Guan, You Lu, Thomas W. Keal, Andrew M. Beale, Alin Marin Elena, C. Richard A. Catlow *Department of Chemistry, University College London

Zeolites and silica polymorphs are central to a range of industrial applications, from emissions abatement to high-pressure structural materials. Here, we present a study employing hybrid QM/MM calculations and machine-learned interatomic potentials (ML-IP) to address silica and zeolite-based chemistry.

First, we investigate the NH_3-SCR mechanism over Cu-chabazite (CHA) [1] and Fe-BEA [2] zeolites. Our hybrid QM/MM simulations [3], supported by DRIFTS experiments with modulation excitation spectroscopy, reveal that water- and ammonia-solvated Cu sites promote the formation of key nitrate intermediates, while also inhibiting reduction steps in the catalytic cycle. Additionally, we extend this approach to Fe-BEA, finding more exothermic formation of crucial intermediates when framework Fe^{3+}/Fe^{2+} is present, indicating enhanced redox properties compared to Al-based frameworks. The synergy in bimetallic Cu–Fe systems offers further insight into optimising zeolite-based catalysts for efficient NO_x reduction. In parallel, we apply the MACE-MP-0 machine-learned potential to model the framework energetics of siliceous zeolites and explore high-pressure phase transitions in silica [4]. Unlike classical potentials that require re-parameterisation, the MACE approach accurately describes structures with varying coordination of Si. Our simulations reproduce the metastability of microporous phases relative to α-quartz and capture the compression behaviour of quartz, coesite, and stishovite. The predicted transition pressures (~3.5 GPa for quartz→coesite and ~9 GPa for coesite→stishovite) align closely with the experiment, demonstrating the reliability and versatility of this ML-based methodology.

Together, we show how multi-scale computational tools can provide robust insight into both the catalytic and structural properties of silica-based materials, enabling the design of more effective zeolite catalysts and enhancing our understanding of silica polymorph stability under extreme conditions.

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An exploration of molecular structures and reaction pathways using adaptive learning and neural networks

Vanda Glezakou, Oak Ridge National Laboratory

Computer simulations, modern algorithms and data science have elevated our ability to better understand chemical structure, reactivity and reactive pathways. Determining transition states in large molecular models still constitutes a computational challenge due to the increasing number of comparable configurational isomers and intermediates.

In my presentation, I will summarize our recent work in developing a computational protocol that explores minima and intermediates on a potential energy surface through an adaptive learning global optimization process. For a given reactive scheme, once a set of low-lying reactants and products is identified, generative adversarial networks (GANs) are used to connect a given set of initial and final states. For example, an ensemble of N reactant and M product states can potentially lead to up to NxM reactive processes and associated transition states. GANs are able to identify energy barriers connecting reactants and products at a fraction of the computational cost, facilitating the discovery of reaction pathways, the construction of kinetic models and extraction of descriptors of reactivity.

Examples from the literature and our current research will be also presented and discussed.

Interfacial Concentration Enhancement and Heterogeneous Nucleation in Non-agitated Urea Solutions

Samira Anker, University of Sheffield

Heterogeneous nucleation is a dominant mechanism of crystal formation, but limited understanding of the role played by solution interfaces is a barrier in the efficient development and control of crystallisation processes. Recent molecular dynamics (MD) simulations observed an interfacial concentration enhancement for systems with experimentally enhanced nucleation rates.

In this work, nucleation experiments and atomistic molecular dynamics (MD) simulations of aqueous urea solutions are performed in the presence of air, glass, diamond and PTFE surfaces. The surfaces are modelled with a Lennard-Jones potential, to reduce the computational resources required, we present a workflow for obtaining these parameters based on atomistic structures.

The MD simulations were used to obtain density profiles and the preferred molecular orientation of urea near the surfaces. Concentration enhancement was observed at the solid surfaces, this was greatest for diamond followed by PTFE and glass. The urea molecules were found to be aligned along the same axis in the interfacial region.

We propose that interfacial concentration enhancement and local molecular ordering lead to lower nucleus-solution interface energy and increased attachment rate of solute molecules to crystal nuclei. This contrasts with classical theories of heterogeneous nucleation that are based solely on bulk solution properties. Our insight will lead to better understanding of nucleation and guide the design of interfaces for improved control of crystallisation processes.

Sensible Asymmetric Units for Crystal Exploration

Jordan Dorrell, University of Southampton

Random structure searching (RSS) methods are simple but low-cost approaches for crystal structure prediction (CSP) that have been widely implemented to great success.[1] In the latest blind test, 13 of the 22 groups which competed in the structure generation portion of the test applied RSS in some form.[2] However, as a brute-force method, traditional RSS is not well equipped to deal with crystals with a large number of symmetry-independent species.

The cost of energy calculations scales with the number of atoms in the unit cell, the number of required geometry optimisation iterations typically increases with the number of independent species in the unit cell, and the number of unique minima on the landscape also increases with the number of independent species in the unit cell. As a modification to RSS for molecular CSP, I will introduce Sensible Asymmetric Units for Crystal Exploration (SAUCE). Instead of individually placing each molecule (quasi) randomly in the asymmetric unit, SAUCE places a single cluster of molecules which are sourced from a minimised crystal.

Compared to traditional RSS implementations, the molecules in crystals generated by SAUCE are in a more energetically favourable environment, and the crystals are denser, leading to faster geometry optimisations, and lower energy minima.

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Vibrations, diffusions, and currents (oh my!) - Unmixing the mechanisms of heat transport in liquids

Cillian Cockrell, Nuclear Futures Institute, Bangor University

Much progress has been made towards understanding the mysterious liquid state in recent years. Microscopic theories resolving the thermodynamic properties of liquids in terms of collective modes (likened to the phonons of solid state physics) have been enormously successful. In particular, liquid heat capacity is determined uniquely by the mean free path of transverse phonons. Transverse phonons in liquids are scattered by atomic diffusion events, which macroscopically amounts to the continuum flow of matter. The more viscous a fluid, the less frequently transverse phonons are scattered, and (all else being equal) the greater its heat capacity. Likewise, a more inviscid fluid has a shorter mean free path and a lower heat capacity. The thermodynamics and transport of liquids therefore share an interesting interrelationship.

The transport of heat, on the other hand, is considerably more complex. We recall the two mechanisms of heat transport: conduction and convection. Unlike shear momentum, matter advects heat as it flows. Conduction describes the “intrinsic” transfer of heat, driven by gradients of temperature. The lattice thermal conductivity of solids is still admissible to phonon theories, with scattering events acting to reduce the conductivity, as they reduce the viscosity of liquids. In liquids, where the dominant mechanism of scattering is atomic mobility itself, a confounding factor is introduced – when an atom is displaced, it takes energy with it. This introduces a competition where atomic displacement impedes vibrational heat transport but facilitates hydrodynamic heat transport.

The waters are further muddied in fluid mixtures, where, even in a barycentric frame, partial mass currents advect heat in a seemingly non-conductive way.

Here, we shall examine these competing mechanisms of heat transport in molecular dynamics simulations of several molten salt systems, whose strong interactions and large mass ratios make analysis delightfully complicated indeed. This causes us to question what we mean by conduction, and how best to assign transport coefficients to atomistic trajectories. Understanding these systems is rather pressing – their thermodynamics and transport properties are of great practical relevance due to the candidacy of molten salts as energy storage media, pyroprocessing hosts, and coolant and fuel carrier fluids in molten salt nuclear reactors. Strongly interacting fluids such as molten salts, and the extent to which their properties are governed by phonons, serve as important and fascinating milestones of how much progress has been made in understanding liquids and how much work remains to be done.

Walking the Edge: Developments in Integrated Materials Design for Alternative Energy Technologies

Denis Kramer, Helmut Schmidt University

Abstract to follow

Molecular quantum materials from first principles

Bo Peng, University of Cambridge

Recent synthesis of molecular networks [1,2] opens new opportunities to study their quantum behaviours. Building upon our previous work on stability [3], chemical functionality [4], and tuneability [5-10] of molecular networks, we show three key aspects of quantum behaviours in molecules for an umbrella of applications from quantum timekeeping to quantum bit and to quantum simulations:

(1) Do quantum states exist in molecules?

(2) How to control quantum states in molecules?

(3) Can we observe new quantum phenomena in molecules?

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Microscale reaction mechanism for ammonia combustion and NOx control

Xizhuo Jiang, Northeastern University (ONLINE)

Ammonia (NH3) is a promising substitute for fossil fuels to achieve the net-zero emission targets. To improve the combustion performance of NH3, assisted methods, such as adding reactive fuels and applying external field, are used in the NH3 combustion.

In the present study, the combustion of NH3 in the presence of methane (CH4), hydrogen (H2) and an electric field is investigated via reactive force field molecular dynamics. The reaction pathways for nitrogen oxides (NOx) generation were identified, and methods to mitigate NOx emissions were proposed.

This study unveiled the mechanism via which the reactive fuels and electric field affect the NH3 combustion performance from an atomic perspective. The findings will be useful for the design of high-efficiency and low-emission combustion chambers in ammonia-powered energy systems.

Electronic Structure and Vibrational Surface Dynamics of Fluorine-Induced Defects on Silicon

Sam Ginzburg, University of Cambridge

Recent first-principles molecular-dynamics investigations into radical-mediated oxygen difluoride adsorption on the monohydrogenated Si {001} (2×1) surface [1] revealed the formation of a cationic Si–H–Si

bridge motif, consistent with three-centre two-electron bonding. A complementary anionic Si–Si–F motif was also identified, consistent with three-centre four-electron bonding. Building on this work, we have performed first-principles electronic-structure calculations and additional molecular-dynamics simulations to explore in detail these and other fluorine-induced surface defects on the same surface.

Our results reveal distinct localised defects within the band gap and metastable states that arise

upon charge variation. We characterise these defects through computed unfolded band structures and vibrational densities of states and discuss their implications for surface transfer doping of silicon thin films.

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Tuning Electronic Structure of Infinite-Layer Nickelate NdNiO2 through Interlayer Spacing

Hangbo Qi, University College London

Since the discovery of superconductivity in infinite-layer nickelates, extensive research has been devoted to uncovering the underlying mechanisms of this phenomenon.

Here, combining density functional theory and Wannier functions calculations, we show that increasing the interlayer spacing of Nd-NiO2 enhances the Ni eg orbital polarization and effective Ni dx2-y2 nearest-neighboring hopping while suppressing the hybridization between Ni dx2-y2 and interstitial s orbitals. This leads to a more two-dimensional electronic structure, which may be favorable for superconductivity. Furthermore, the interlayer spacing strongly affects the Fermi surface topology and the pocket size around A point, i.e., the self-doping effect. Given that the self-doping effect is considered a key feature distinguishing nickelates from cuprates, this may help explain why the superconducting transition temperature of cuprates is higher.

Our results highlight the critical role of interlayer spacing in tuning the electronic structure of infinite-layer nickelates and suggest a feasible route to optimizing superconductivity through structural engineering.

Materials Discovery with Ephemeral Data Derived Potentials

Peter Cooke, University of Cambridge

The development of Machine Learned Interatomic Potentials (MLIPs) has revolutionised atomistic simulations over recent years. MLIPs enable simulations with accuracy comparable to quantum mechanical approaches at up to 10 million times smaller computational cost. The ephemeral data derived potentials (EDDPs[1,2]) are a flexible class of MLIP that can utilise comparatively small neural networks for fast and accurate simulations.

Materials discovery techniques, such as random structure searching, can exploit this acceleration in a number of ways. Larger system sizes and chemical spaces can be explored, or more computationally intensive structure optimisers, utilising molecular dynamics, can incorporated[3].

Through a range of applications, we demonstrate that more complex optimisers can improve search performance for large systems. Through example simulations in LAMMPS[4], we further show that the EDDPs can be employed beyond structure searching, to explore complex dynamical behaviour across a range of conditions and chemical systems.

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A multiscale workflow from the atomistic level to simulations of entire batteries

Alberto Hernandez-Melian, University of Southampton

The Doyle-Fuller-Newman (DFN) model [1] uses conservation laws to describe the electrochemical reactions at the interface between solid and electrolyte in a battery, allowing for accurate simulation of its performance through multiple charge and discharge cycles. The open-source PyBaMM library [2] provides an accessible implementation of this model using Python, including a configurable interface and values for the many parameters involved. Experimental measurements are usually employed to obtain these values, but not all are easily accessible and so in some cases a complementary first-principles approach would be desirable, where atomistic simulations are used to inform battery behaviour at larger length scales. This approach could improve the predictive capability of the models and is transferable to other materials (e.g. Na-ion batteries, etc).

We present our work using different quantum atomistic simulation methods to compute lithium diffusion coefficients in graphite at different concentrations and temperatures, which are then employed in PyBaMM calculations. We use the DFTB method [3] as implemented in ONETEP [4], a code for large-scale quantum atomistic simulations of complex systems, and the MACE-MP-0 [5] machine learned interatomic potential and compare their effectiveness. Our aim is to extend this methodology to more parameters, creating a multiscale workflow that can improve the accuracy and simplify the running of all battery simulations.

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Stabilising Polarisation in Ultrathin Ferroelectric Films: The Role of Surface Hydrogen Coverages

Nisrine Sakaki, London South Bank University

Ferroelectric materials are a class of materials that exhibit spontaneous electric polarisation, which can be reversed by an external electric field. This unique property makes them ideal for a wide range of applications, including memory devices, sensors, actuators, and capacitors. Ferroelectric materials, such as lead titanate ($PbTiO_3$) and barium titanate ($BaTiO_3$), are of particular interest due to their high polarisation and the ability to tailor their properties for specific applications.

The polarisation behaviour in these materials is highly sensitive to external factors such as strain, temperature, and surface modifications. One such modification is the deposition of hydrogen atoms on the surface, which can significantly influence the polarisation value and direction. This research investigates the effect of hydrogen deposition on ferroelectric materials, specifically the surface interaction and its role in controlling the polarisation. By varying the hydrogen deposition percentage, we explore how the polarisation can be adjusted, with potential implications for device performance and functionality.

This study provides valuable insights into the mechanisms driving polarisation changes in ferroelectric materials and their applications in modern electronics.

Computational Insights into the Remediation of Endocrine Disruptor Contaminated Water

Sam Shepherd, Queen's University Belfast

Many industrially developed chemicals exhibit unintended biological activity in humans, prompting legislative changes after these effects are uncovered, particularly for those that persist in the environment over extended time periods [1,2]. Whilst this reduced usage is encouraging, it is not retroactive and hence does little to reverse existing contamination. One notable, concerning example is that of endocrine disrupting chemicals (EDCs) like bisphenol-A (BPA) and triclosan (TCS), which interfere with the hormone system and can cause serious health issues [3].

Removing these chemicals from water is difficult and costly, with methods often specific to certain EDCs and ineffective for others. This difficulty is only exacerbated as more chemicals are found to possess endocrine disrupting properties. Experimental methods can be complemented by computational approaches, which offer more flexible screening options and can reveal detailed insights into the mechanisms of removal, allowing for broader generalisations to other contaminants to be obtained [4].

In this direction, we conducted molecular dynamics simulations on the adsorption of various EDCs onto carbon nanotubes and organo-modified montmorillonite. Using metadynamics, we are able to obtain values for the free energies of adsorption, as well as the lifetime of the adsorption complex. We find that both the presence of heteroatoms within the EDC and the flexibility of the molecule play key roles in the adsorption mechanism on the nanotube, while the accessibility of the interlayer plays a critical factor when adsorbing onto clay minerals.

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Molecular materials: From accurate numbers to detailed chemical insight

Felix Plasser, Loughborough University

Molecular materials provide a highly promising new design space for the development of solar cells, light sources, and batteries. Tremendous effort is invested in developing optimized molecules for these applications. Computational methods have become in many cases powerful enough to provide accurate numbers and, thus, accurately predict the properties of interest. However, new challenges come into play when interpreting the results of the computations in order to obtain general chemical insight and, ultimately, develop new design guidelines.

It is the purpose of this talk to present our computational tools (1,2) allowing to gain detailed insight even from challenging computations on complex systems and to illustrate the further path of developing general design rules. To date only a small number of design rules exist, mostly based on the energies and shapes of the frontier molecular orbitals (FMO), meaning that extensive screening is often necessary. It is the purpose of this work to highlight two alternative strategies, going beyond the standard FMO picture, to explain photophysical behaviour and ultimately design new molecules: (i) modulation of singlet-triplet gaps via the transition density, and (ii) tuning of excitation energies via excited-state aromaticity.

This talk will first address the development of new design rules for materials with large singlet-triplet gaps, as are needed for singlet fission solar cells. Previously, we have shown that the transition density provides an intuitive way for explaining, both, optical brightness and singlet-triplet gaps (3). Applied to the case of singlet fission, this framework was used to devise three now rules for maximizing S1/T1 gaps: (i) reducing the number of p-electrons, (ii) localizing the excited electrons within the p-system, and (iii) optimizing specific through-space interactions (4, 5). We highlight the applicability of this model bridging from simple hydrocarbon backbones to realistic dyes. As a second example, we will investigate the optical properties of bridged p-conjugated diradicals. Firstly, we will discuss the different types of diradical, zwitterionic and charge-transfer states that are accessible in these systems (6).

Using this framework, we will explain the unexpected absorption and luminescence properties of a cyclopenta-dithiophene bridged tris (2,4,6 trichlorophenyl) methyl (TTM) diradical (7).

Calculating system properties on the fly in DL_POLY 5

Harvey Devereux, Queen Mary University of London

Performing calculations on-the-fly can confer performance advantages by eliminating the need to save data or perform input/output operations at runtime. Such algorithms operate by sequentially updating their state as new data arrive. This paradigm, also termed “online algorithms”, is ubiquitous in the analysis of big data streams. In molecular dynamics the system trajectory, mapping atomic configurations through simulation time, is an example of such a data stream where analysis after the fact remains a common paradigm. Such an approach in large scale systems, e.g. reaching 1 billion atoms (length scales of 1 μm) is infeasible. By casting standard analysis of system trajectories as online algorithms, we can eliminate trajectory storage, whilst still producing detailed analysis of the simulation.

In DL_POLY 5, we have implemented a general framework for calculating arbitrary correlation functions of simulation data on-the-fly with no trajectory storage. We support commonly used system properties such as atom and rigid body velocities, rigid body orientational velocities, stress, heat flux, as well as k-space currents, densities and stresses. Alongside basic statistics such as system volume, temperature and pressure. Using these we are able to calculate for example the viscosity and thermal-conductivity, elastic constants, and velocity auto-correlation functions, as well as intermediate scattering functions and dynamical structure factors without trajectory storage.

Our implementation in DL_POLY 5 is designed to be highly extensible to new simulation properties. Which we continue to develop, for example targeting general flexible molecules and molecule components (bonds, angles, etc.). Additionally for a user, we allow the combination of any components of supported correlatable quantities into user defined correlations in the CONTROL file.

Update from MMM Hub partners HPE & Intel

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Abstract tbc

Hydrogen-Mediated Electronic Modulation in Monolayer Channel Interfaces for Protonic Neuromorphic Devices

Vasileios Fotopoulos, Massachusetts Institute of Technology

Electrochemical random-access memory (ECRAM) devices have emerged as a novel type of programmable resistor for crossbar arrays, one of the most promising architectures for implementing energy-efficient artificial neural networks. ECRAMs consist of three key functional layers: an ion reservoir, a solid electrolyte, and a channel. Through voltage-driven intercalation of mobile ions (e.g., H^+), the electronic conductivity of the channel can be finely modulated, enabling precise control over the resistance state of the device. The operating speed and energy efficiency of ECRAMs critically depend on ion mobility in the electrolyte and channel materials, as well as interfacial transfer properties. Mixed ionic and electronic conducting oxides, such as WO_3, have been previously investigated as channel materials. However, their bulk nature necessitates 3D ion redistribution, leading to undesirably long conductivity settling times. In contrast, 2D materials, including monolayers (MLs) of transition metal dichalcogenides (TMDs; e.g., MoS_2), offer a promising alternative, but the interfacial ion diffusion characteristics and their impact on conductivity remain underexplored.

This work employs Density Functional Theory (DFT) to study H incorporation and diffusion at interfaces between solid electrolytes (e.g., SiO_2) and ML 2D channel materials. We identify the most stable incorporation sites and the effects of incorporation on the electronic structure of the channel. Additionally, we explore the influence of various SiO_2 surface terminations, including oxygen-terminated, silicon-terminated, and reconstructed surfaces with unsaturated or fully saturated Si and O bonds. For MoS_2 channels, the SiO_2 surface termination significantly affects both the charge state and the most stable incorporation site of H. Surfaces with fully saturated bonds enable barrier-free diffusion of H from the electrolyte to the channel. Once incorporated onto the MoS_2 surface, H induces n-type doping, leading to an increase in the channel's conductivity.

By assessing the electronic interactions between H and 2D channel materials, this work identifies optimal surface termination and material combinations to enhance ion migration and conductivity modulation, contributing to the development of high-performance, energy-efficient neuromorphic computing hardware.

Strong electron correlations in Novel Battery materials

Andrew Morris, University of Birmingham

The lithium nickel manganese cobalt oxides, LiNixMnyCozO2 (x+y+z=1) (NMC) are a promising family of materials for the cathodes of lithium-ion batteries (LIB). The Ni-rich NMCs especially, exhibit excellent performance as high-voltage cathode materials, enabling batteries with high energy densities and high capacities of around 200- 275mAh/g. However, Ni-rich NMCs are prone to structural instabilities and oxygen loss leading to electrode degradation, a hurdle that must be overcome before widespread commercialisation. However, for describing the crystal and electronic structure of NMCs, DFT falls short due to a lack of ability to account for strong electron correlations.

I introduce the more advanced dynamical-mean-field theory (DMFT) and show that it correctly describes the electronic properties of the NMC family. This, in turn allows us to uncover the mechanism of oxygen loss on delithiation of NMC. Density-functional theory (DFT) is now the standard modelling technique for atomistic physics, chemistry and materials science. It allows us to solve a single-particle Schrödinger-like equation for the energies of electrons in molecules and solids, thereby allowing us to deduce the material's crystal structure and properties. I introduce DFT and show how it can clarify the complex behaviour of a class of LIB cathodes, the tungsten niobates. Indeed, this behaviour may then be rationalised within the much simpler crystal-field theory.

A static reformulation of the GW approximation through conservation of spectral moments

Marcus Allen, King's College London

Due to their ability to compactly encode quasiparticle excitation spectra, Green's function-based methods have become a crucial tool in understanding reaction mechanisms and optoelectronic properties. The GW approximation has risen to prominence due to its cost-efficient manner to describe single-electron excitation spectra. We consider a full frequency GW implementation focused on an 'upfolded' or Hamiltonian representation of the dynamical Green's function, whereby the correlation-driven changes are induced by coupling to external degrees of freedom.

Our novel approach conserves the GW self-energy only up to a desired order of static spectral moments of its dynamical distribution. This avoids the requirement for a frequency or time grid, allowing for a zero temperature spectra to be obtained from a complete application of Dyson's equation. Through this upfolded approach calculations are systematically improvable though increasing the number of moments while also providing novel opportunities for self-consistency.

Our GW implementation equally treats excitations for molecules and solids with competitive scaling seen across broad benchmarks for both types of systems. Encouragingly, this method applied to the 137-atom Chlorophyll-A was computationally efficient while providing the full-frequency quasiparticle spectra at zero temperature from a single-shot.

Accelerating the energy transition via highly selective materials: an overview of molecular, multiscale and AI model

Grazia De Angelis, University of Edinburgh

Advanced selective materials are crucial to enable the energy transition and achieving Net Zero targets, in hydrogen production as well as in CO2 capture and conversion, and development of biodegradable plastics.

I will present examples of multiscale modelling techniques, encompassing molecular modelling, macroscopic tools and AI that connect the macroscopic selective performance of advanced separation materials to their molecular structures, paving the way for the digital design of groundbreaking polymer chemistries.

In hydrogen storage and transport, we've created a multiscale model that simulates the microstate of semicrystalline polymers at the molecular level, feeding into larger-scale simulations to predict material performance based on chemical properties.

For CO2 capture, we have developed a method that predicts the performance of polymeric membranes in capturing CO2 from their monomeric molecular structures, using Machine Learning paired with Lattice-Fluid equations of state.

In biopolymer development, our refined multiscale model links atomistic and macroscopic thermodynamic calculations, allowing us to forecast the barrier performance of various formulations with minimal experimental input, thus speeding up the development of new, sustainable polymers.

AWE Materials Modelling for Ageing and Lifetime Predictions

Matt Darby, AWE

For 75 years, AWE has proudly played a role of critical national importance: helping deliver the UK’s nuclear deterrent. We are at the forefront of nuclear technology and innovation, from delivering the warheads for the UK’s Continuous At Sea Deterrent (CASD), to developing novel solutions to deter threats and support counter terrorism activities – always delivering to keep our nation safe and secure. AWE has pioneered advancements in nuclear science and technology in areas including physics, engineering, materials science, and high-performance computing. Together we’ve helped shape the UK’s technological landscape, driving innovation that extends well beyond defence.

An exciting aspect of innovation at AWE is in the use of modelling to provide predictive capabilities to underwrite performance, manufacture and ageing of a broad variety of materials from actinides to explosives. In this talk, we will explore the key computational techniques employed by our Group at AWE to investigate the behaviour of a variety of materials, highlighting how a modelling and simulation-based approach is advancing our understanding of complex material systems. We will discuss models constructed using a range of different computational techniques, from electronic structure theory to finite element modelling. We will demonstrate how AWE applies these methods to different problems in materials science, and how we bridge length scales to seamlessly integrate modelling with experiment.

Voltage-Driven Evolution of Lithium Nanoparticle Morphology

Brad Ayers, University of Southampton

Lithium metal anodes present a promising avenue for next-generation energy storage, yet their practical implementation remains hindered by uncontrolled morphological evolution during normal battery operation, particularly dendrite formation.

To address this challenge, we systematically investigated the voltage-dependent evolution of lithium nanoparticle morphology within battery-relevant electrolyte environments using grand canonical density functional theory (GC-DFT) [1]. This computational framework enables direct quantification of the interplay between applied potential, surface energetics, and resulting crystal shape transformations.

Our comprehensive analysis of thirteen crystallographically distinct Li surfaces reveals fascinating insights into their electrochemical behaviour. Notably, solvation effects induce subtle yet significant redistributions in relative surface stability, with higher-index facets becoming preferentially stabilised through efficient screening.

Building upon these findings, we observed morphological transformations as the increasingly negative potentials were applied. The lithium structures transition towards rhombic dodecahedral formations dominated by {110} facets, with the contribution of these facets to the overall surface area increasing dramatically ”from 29.7% to 100%”as potential decreases from -1.0 V to -1.75 V vs Li/Li+. This structural evolution is accompanied by a substantial reduction in surface energy, decreasing from 0.445-0.480 J/mÂ² to 0.210-0.230 J/mÂ².

These theoretical predictions align excellently with recent experimental observations by Yuan et al. [2], who demonstrated that lithium naturally adopts rhombic dodecahedral morphology bounded by {110} facets under conditions where deposition kinetics outpace solid electrolyte interphase formation. This complementarity between computational and experimental approaches provides compelling evidence that the rhombic dodecahedron represents the fundamental equilibrium shape for lithium metal under electrochemical conditions.

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First Principles Calculations of Temperature Dependent Exciton Binding Energies and Dissociation Rates in Semiconductors and Insulators

Marina Filip, University of Oxford

In this talk, Marina will present a recent first principle framework that have been developed to understand the impact of ionic vibrations on the binding energy, fine structure and dissociation of excitons in semiconductors and insulators[1,2]. Our new framework builds upon standard state-of-the art Bethe-Salpeter Equation [3], and includes the effect of ionic vibrations at the level of the electron-hole interaction kernel.

Marina will first introduce the theoretical background of this approach, from the point of view of scattering theory [4]. Furthermore, Marina will describe the implementation and discuss its applications to several examples of semiconductor and insulators studied recently [4-5]. These applications will be discussed, starting from model theoretical approaches within the Wannier-Mott and Frohlich models, followed by direct and fully converged first principles calculations of exciton binding energies and dissociation rates for binary and ternary semiconductors andinsulators [1,2,4,5].

The talk will show how the recently developed framework allows for compute temperature dependent exciton binding energies and exciton dissociation rates with good accuracy, and trends in agreement with experimental measurements.

Posters

1	**Marcus Allen** King's College London	A static reformulation of the GW approximation through conservation of spectral moments
2	**Samira Anker** University of Sheffield	Framework for Predictive Modelling of Segregation at Grain Boundaries
3	**Joan Clark-Nicolas** University of Lincoln	Practical Workflows for High-Throughput CP2K Simulations with pycp2k
4	**Harvey Devereux** Queen Mary University of London	Elastic constants, k-space currents, and correlations on-the-fly in DL_POLY
5	**Jordan Dorrell** University of Southampton	Sensible Asymmetric Units for Crystal Exploration
6	**Alberto Hernandez-Melian** University of Southampton	A multiscale workflow from the atomistic level to simulations of entire batteries
7	**Syed Jawad Hussain** Peking University	A High-Performance Solid-State Electrolyte Na_4ZrF_8 with Exceptional Ionic Conductivity and Electrochemical and Interfacial Stability
8	**Darren Lim** University of Cambridge	The graphene-water contact angle from machine learning interatomic potentials
9	**Bo Peng** University of Cambridge	Molecular quantum materials from first principles
10	**Peter Tsioumparakis** University of Southampton	Simulating Oxygen adsorption onto Platinum PEM Hydrogen fuel cell electrocatalysts
11	**Yee Chit Wong** University of Warwick	First-Principles Defect and Migration Barrier Studies of Correlated Oxides with Machine Learning Perspectives
12	Brad Ayers University of Southampton	Voltage-Driven Evolution of Lithium Nanoparticle Morphology
13	Sam Shepherd Queen’s University Belfast	Computational Insights into the Remediation of Endocrine Disruptor Contaminated Water