



MATERIALS AND MOLECULAR MODELLING HUB

Conference & User Meeting 2024

Programme & Abstracts

MMM Hub Conference & User Meeting Organising Committee

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Sponsors



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Programme

13:30, Tuesday 29th October 2024 – 12:30, Thursday 31st October 2024, Battle of Britain Bunker, Wren Avenue, Uxbridge, UB10 0GG

Tuesday 29th October

- 13:30 – 14:00 **Registration and refreshments**
- 14:00 – 14:10 **Welcome – George Booth, King's College London**
- 14:10 – 14:40 **Gabor Csanyi, University of Cambridge**
A force field for the periodic table
- 14:40 – 15:00 **Sam Shepherd, Queen's University Belfast**
Digging into the detail; Discrepancies in the fine structure of kaolin minerals as described by dispersion corrected DFT
- 15:00 – 15:20 **Kemal Atalar, King's College London**
Fast and accurate nonadiabatic molecular dynamics through variational wavefunction interpolation
- 15:20 – 15:50 **Refreshments**
- 15:50 – 16:10 **Mauricio Cafiero, University of Reading**
Transformer-based GPT models for creating virtual screening libraries of molecules with tuned properties
- 16:10 – 16:30 **Joan Clark-Nicholas, University of Lincoln**
Machine Learning-Driven Molecular Dynamics Simulations for Chemical Reaction Exploration
- 16:30 – 16:50 **Carlos Corral-Casas, Imperial College London**
Molecular Insights into the Adsorption of Detergent Additives on Carbonaceous Deposits from Hydrocarbon Fuels
- 17:20 **Close of Day 1**

Wednesday 30th October

- 10:00 – 10:30 **Tea, coffee, pastries & fruit**
- 10:30 – 10:50 **Shivani Grover, University of Edinburgh**
Choline based plastic crystals as barocaloric materials: insights from ab initio molecular dynamics
- 10:50 – 11:10 **Nabil Menai, Bristol University**
Optimizing Spin Hall Angle in Mn-based Antiferromagnetic Alloys
- 11:10 – 11:40 **Juliana Morbec, Keele University**
Exploring hybrid organic/2D van der Waals heterostructures with first-principles quantum mechanical simulations
- 11:40 – 12:00 **Yao Wei, King's College London**
Global Optimization of Molybdenum Subnanoclusters on Graphene: a Consistent Approach Towards Catalytic Applications

- 12:00 – 12:20 **Refreshments**
- 12:20 – 12:40 **Ingvars Vitenburgs, Imperial College London**
Extended Coupled Cluster approach to Twisted Graphene Layers
- 12:50 – 13:10 **Christopher Tat Shun Cheung, Imperial College London**
Coexisting charge density waves in twisted bilayer NbSe₂
- 13:10 – 13:40 **Adam Roe, Intel / Hewlett Packard Enterprise (HPE)**
HPE introduction with an Intel Technology Update, with a focus on Xeon Max and Future Xeon Processors
- 13:40 – 14:40 **Lunchbreak**
- 14:40 – 15:00 **Cyril Xu, University College London**
Theoretical Investigations on Point Defects in Energy Materials Using a Mott-Littleton Method
- 15:00 – 15:30 **Devis Di Tommaso, Queen Mary University of London**
Identifying CO₂ Conversion Catalysts: High-Throughput DFT Calculations, Machine Learning, and Beyond
- 15:30 – 16:10 **Flash talk session**
- Marcus Allen, King's College London
A novel 'moment'-based GW algorithm for molecules and solids
- Wenxuan Cai, Imperial College London
Modelling core electron binding energy of metal oxides
- Dominique de Jong-Hoogland, King's College London
Computational Investigation of the Effect of BODIPY Labelling on Peptide-Membrane Interaction
- Merve Dene, University of Reading
Understanding the Hexagonal Boron Nitride / Re (0001) Interface: Experimental and Computational Analysis
- Basil Ibrahim, King's College London
Spectral functions from a Green's function embedding
- Miguel Luque Canete, King's College London
Phonon-limited conductivity of topological surface states in Bi₂Se₃ and graphene
- Frances Towers Tompkins, University of Reading
Anion-Dependent Strength Scale of Interactions in Ionic Liquids: XPS and AIMD
- Matteo Valderrama, Imperial College London
Beyond Graphene: Computational Screening of 2D Materials to Eliminate Friction

Chengcheng Xiao, Imperial College London
Brillouin zone sampling in ONETEP

Chin Yong, STFC
D_ATA (Atom Typer and Analyser) – a new software to investigate atomic interactions

16:10 – 17:40 **Poster Session / Drinks reception**

18:30 – 20:30 **Dinner at Bella Italia, Uxbridge**

Thursday 31st October

10:00 – 10:30 **Tea, coffee, pastries & fruit**

10:30 – 10:50 **Cillian Cockrell, Bangor University**

Fast dynamics and high effective dimensionality of liquid and supercritical fluidity

10:50 – 11:10 **Andras Petho, University College London**

Investigating the conductive properties of multi-heme cytochromes

11:10 – 11:40 **Carole Morrison, University of Edinburgh**

The (other) big bang theory: towards a structure/property model to rationalise the impact sensitivities of energetic materials

11:40 – 12:00 **David Wilkins, Queen's University Belfast**

Machine Learning of Polarisation: Problems and Solutions

12:00 – 12:00 **Alessandro Santana Bonilla, King's College London**

Unlocking Conjugated Polymers' Potential: A Data-Driven Approach using PySoftK

12:30 **End**

A force field for the periodic table

Gabor Csanyi - **University of Cambridge**

A new computational task has been defined and solved over the past 15 years for extended material systems: the analytic fitting of the Born-Oppenheimer potential energy surface as a function of nuclear coordinates. The resulting potentials (“force fields”) are reactive, many-body, with evaluation costs that are currently on the order of 0.1-10 ms/atom/cpu core (or about 1-10ms on a powerful GPU), and reach accuracies of a few meV/atom when trained specifically for a given system using iterative or active learning methods.

The latest and most successful architectures leverage many-body symmetric descriptions of local geometry and equivariant message passing networks. Perhaps the most surprising recent result is the stability of models trained on very diverse training sets across the whole periodic table. Our recently discovery is that the MACE-MP-0 model that was trained on just ~150,000 real and hypothetical small inorganic crystals (90% of training set < 70 atoms), is capable of stable molecular dynamics at ambient conditions on any system tested so far – this includes crystals, liquids, surfaces, clusters, molecules, and combinations of all of these.

The astounding generalisation performance of such foundation models open the possibility to creating a universally applicable interatomic potential with useful accuracy (especially when fine-tuned with a little bit of domain-specific data) and democratise quantum-accurate large-scale molecular simulations by lowering the barrier to entry into the field.

Digging into the detail; Discrepancies in the fine structure of kaolin minerals as described by dispersion corrected DFT

Sam Shepherd - Queen's University Belfast

Clay minerals are complex, naturally occurring layered materials whose unique structures allow them to be used in processes where they act as catalysts or highly selective adsorbents. However, accurately describing the interactions which take place within and between the layers of clay minerals remains a challenge which limits our understanding of the potential of these minerals.

When studied theoretically, the need for an accurate description of dispersion interactions is well understood, but accounting for the necessarily large system sizes, long timescales and physical complexity needed to observe the processes of interest has hitherto limited theoretical study into these minerals.

To rectify this, we created a suite of machine learned interatomic potentials (MLIPs), trained using DFT level calculations with different descriptions of dispersion interactions. We used these potentials to overcome the computational expense of simulating these minerals at this level of theory and have studied the kaolin minerals for extended timescales. Thus, we have been able to study the structural and dynamical properties of kaolinite, dickite, and nacrite with previously unachievable levels of physical detail.

We find that different dispersion corrections yield a surprisingly different description of the polyhedral units of the clay layers, and a vastly different description of the interlayer dynamics of the different kaolin polymorphs. We use path integral molecular dynamics to discuss the necessity of nuclear quantum effects when considering these interactions and conclude that they are vital to the description of interlayer dynamics in kaolin minerals.

Fast and accurate nonadiabatic molecular dynamics through variational wavefunction interpolation

Kemal Atalar - King's College London

The coupling of excited electronic states to atomic motion is key to addressing challenges in photochemistry and photophysics. The computational study of these states, however, is hindered by the prohibitive cost of the multi-state electronic structure calculations for numerous atomic configurations, in addition to gradients and the coupling between states. This leads to the adoption of approximate methodologies that underestimate or ignore electronic correlation while limiting the timescales accessible.

To overcome these limitations, we extend eigenvector continuation [1] to develop an efficient multi-state method that interpolates a small training set of ab-initio many-body wavefunctions across nuclear phase space at mean-field cost. [2] This is accomplished through a variational ansatz within the subspace defined by a few training eigenstates, rendering all chemical properties along a dynamical trajectory accessible and enabling efficient simulation of nonadiabatic molecular dynamics (MD). We also introduce an active learning scheme that ensures a compact and systematically improvable training set. We apply this approach to the nonadiabatic MD of a photoexcited 28-atom hydrogen chain, uncovering surprising complexity in its nuclear motion. With just 22 DMRG calculations, we infer multi-state energies, forces, and nonadiabatic couplings at 12,000 geometries with high accuracy along molecular trajectories—a task infeasible with a brute-force approach.

Our work bridges the gap between accurate single-point electronic structure methods and the timescales relevant to photo-induced molecular dynamics.

[1] Y. Rath and G. H. Booth, arXiv:2402.11097 [physics.chem-ph]; [2] K. Atalar, Y. Rath, R. Crespo-Otero and G. H. Booth, Faraday Discussions, 2024

Transformer-based GPT models for creating virtual screening libraries of molecules with tuned properties

Mauricio Cafiero – University of Reading

Several generative, pre-trained models were developed to create virtual screening libraries of molecules with affinity for the HMG Coenzyme A reductase (HMGCR) enzyme. These models were pre-trained on general drug molecule structures and then fine-tuned to create HMGCR inhibitors.

The balance of pre-training and fine-tuning transformer blocks were varied from 100% pre-trained/0% fine-tuned to 0% pre-trained/100% fine-tuned to find the proportions that yielded the most desirable molecule sets. Molecule libraries were generated with two “temperatures,” $T=0$, meaning the most probably next token was taken in the generation process, and $T=0.5$, meaning that a less-probably next token could be selected at random. Finally, the number of input token to the generation process was varied to produce the most robust libraries. The libraries were then screened by using a deep neural network trained on HMGCR inhibitors to predict IC50 values and by docking the molecules in the HMGCR binding suite. Other screens included docking, Tanimoto similarity and synthetic accessibility scores.

The molecules produced by the models were then grouped into clusters using k-means analysis and classified by inspection. It was found that more fine-tuning/less pre-training lead to more potent inhibitors, but less stable models, while less fine-tuning/more pre-training still produced good inhibitors, but were more stable. Prompt/input length into the generative models was also found to have a large effect, with shorter prompts producing more robust libraries. The libraries contained ~42% of molecules that were statin-like according to k-means analysis.

Machine Learning-Driven Molecular Dynamics Simulations for Chemical Reaction Exploration

Joan Clark-Nicholas - University of Lincoln

We present a machine learning-based, molecular dynamics (ML-MD) workflow designed to investigate chemical reactions and identify intermediate states.

The workflow begins with classical molecular dynamics (MD) simulations of both the reactant and product states. From these simulations, we extract snapshots that are subsequently subjected to ab initio calculations to generate descriptors for training an initial machine learning (ML) force field. This force field is then employed to perform the first iteration of ML-MD simulations. Following this, the snapshots obtained from the first ML-MD simulation are subjected to ab initio calculations and their descriptors added to the training set, and the ML force field is retrained. Then the second iteration of ML-MD, with the newly trained ML force field, is started from the reactant snapshot that shows the highest value for a chosen metric of similarity with the product, and vice versa.

After every iteration of the workflow, the chosen similarity metric is used to calculate an approximation to the equilibrium constant, and the workflow is considered complete when the equilibrium constants obtained from the forward and reverse simulations converge towards the same value. We demonstrate the effectiveness of our protocol by applying it to a well characterised chemical reaction.

Molecular Insights into the Adsorption of Detergent Additives on Carbonaceous Deposits from Hydrocarbon Fuels

Carlos Corral-Casas - Imperial College London

Deposits can reduce engine performance and increase emissions, particularly in modern direct-injection engines. Surfactants known as detergent additives are the main mitigation strategy to prevent their formation by keeping their precursors suspended in the fuel.

In this work, we show how molecular simulations can be used to virtually screen the ability of detergents to bind to a major class of deposit precursors, namely, polyaromatic hydrocarbons. We use MD with the ABF method to generate the potential of mean force, as well as density functional theory calculations to validate the force field of choice. We find that a zwitterionic surfactant outperforms conventional non-ionic polyisobutylene succinimide, because of the addition of functional groups that enhance the binding strength.

This approach shows great promise for accelerating the discovery of novel detergents that facilitate more advanced fuel formulations to reduce emissions.

Choline based plastic crystals as barocaloric materials: insights from ab initio molecular dynamics

Shivani Grover - University of Edinburgh

Solid-state refrigeration technologies based on barocaloric effects offer a cleaner alternative solution to conventional refrigeration technologies based on compression cycles of greenhouse gases. Thus, materials with large solid-state caloric effects induced by external field (mechanical, electric or magnetic field) need further investigation and development to realise their full potential [1,2]. In the present work, we explore the potential of choline-based plastic crystals, $(C_5H_{14}NO)_2MX_4$ where $M = Co, Zn, Cu$, and $X = Cl, Br, I$, as promising barocaloric materials due to a large entropy change ($\sim 100 \text{ JK}^{-1} \text{ kg}^{-1}$) associated with the symmetry-breaking disorder-order phase transition.

Using ab initio molecular dynamics as implemented in CP2K, we provide insights into the structural dynamics and hydrogen bonding between the choline and $CoCl_4$ that characterise the two phases. From our calculation of vibrational density of states, we estimate the entropy change across the phase transition. Our model is validated with our experimental study, thus providing a complete understanding of the interplay between dynamic and disordering effects in choline based plastic crystals.

References: 1. Moya, X., Kar-Narayan, S. & Mathur, N. D. Caloric materials near ferroic phase transitions. *Nature Materials* 13, 439-450 (2014). 2. Li, B. et al. Colossal barocaloric effects in plastic crystals. *Nature* 567, 506-510 (2019).

Optimizing Spin Hall Angle in Mn-based Antiferromagnetic Alloys

Nabil Menai - Bristol University

Antiferromagnets (AFMs) were once believed not to show anomalous Hall conductivity (AHC), unlike ferromagnets, known for this effect since 1881. Recently, some AFMs have been shown to exhibit AHC and hold promise for spintronics due to their scalability, robustness to magnetic fields, and ultrafast spin dynamics [1, 2, 3]. Using density functional theory and Green's function methods, we calculate the spin Hall conductivity (SHC) of Mn-based AFM alloys, incorporating intrinsic and extrinsic contributions [4, 5]. We find that doping MnPt with Pd increases the spin Hall angle (SHA) from 1% to 4.1%, and with Ir, the SHA reaches up to 8% at room temperature, suggesting these alloys are ideal for efficient spin current generation.

References

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Exploring hybrid organic/2D van der Waals heterostructures with first-principles quantum mechanical simulations

Juliana Morbec - Keele University

Combining two-dimensional (2D) materials with organic materials can be highly attractive for applications that require flexibility and where size and weight are important parameters, such as in wearable, portable, and mobile devices. Organic materials often exhibit excellent optical absorption efficiency and photo- and temperature-induced conformational changes, while 2D materials tend to demonstrate relatively high carrier mobility, superior mechanical flexibility, and tuneable electronic and optical properties. Combining both systems can stabilize the organic materials and create heterostructures with both high carrier mobility and high optical absorption efficiency, which is promising for solar energy conversion. In this work, we investigate heterostructures composed of organic molecules (e.g., pentacene and azulene) and transition metal dichalcogenides (TMDs) for application in photovoltaic devices, using density-functional-theory calculations. We examine the interaction between the molecules and monolayer TMDs, as well as the band alignment of the heterostructures, considering the effects of molecular coverage, rotation, and dielectric screening.

Global Optimization of Molybdenum Subnanoclusters on Graphene: A Consistent Approach Towards Catalytic Applications

Yao Wei - King's College London

The development of novel sub-nanometer clusters (SNCs) catalysts with superior catalytic performance depends on the precise control of clusters' atomistic sizes, shapes, and accurate deposition onto surfaces. The intrinsic complexity of the adsorption process complicates the ability to achieve an atomistic understanding

of the most relevant structure-reactivity relationships hampering the rational design of novel catalytic materials.

In most cases, existing computational approaches rely on just a few structures to draw conclusions on clusters' reactivity thereby neglecting the complexity of the existing energy landscapes thus leading to insufficient sampling and, most likely, unreliable predictions. Moreover, modelling of the actual experimental procedure that is responsible for the deposition of SNCs on surfaces is often not done even though in some cases this procedure may enhance the significance of certain (e.g., metastable) adsorption geometries. This study proposes a novel systematic approach that utilizes global search techniques, specifically, the particle swarm optimization (PSO) method, in conjunction with ab-initio calculations, to simulate all stages in the beam experiments, from predicting the most relevant SNCs structures in the beam and on a surface, to their reactivity. To illustrate the main steps of our approach, we consider the deposition of Molybdenum SNC of 6 Mo atoms on a free-standing graphene surface, as well as their catalytic properties with respect to the CO molecule dissociation reaction. Even though our calculations are not exhaustive and serve only to produce an illustration of the method, they are still able to provide insight into the complicated energy landscape of Mo SNCs on graphene demonstrating the catalytic activity of Mo SNCs and the importance of performing statistical sampling of available configurations.

This study establishes a reliable procedure for performing theoretical rational design predictions.

Extended Coupled Cluster approach to Twisted Graphene Layers

Ingvars Vitenburgs - Imperial College London

A study of correlation effects in twisted bilayer graphene is presented using the extended coupled cluster method at consistent mean-field and beyond mean-field truncations. In order to describe the phase transitions in this strongly correlated system, equations and a suitable implementation is developed for the method. Combining modern tensor contraction techniques with singular value decomposition, the correlation effects are successfully described in a qualitative manner, with the majority of both short-range and long-range Coulomb interactions included. Superconductivity is derived, analytically, to be possible only when beyond-mean-field correlations are included at non-zero fillings. Furthermore, the superconducting gap is found to peak at an angle $\theta_c = 1.00^\circ$ with a BCS value for the critical temperature of $T_{\text{c}}^{\text{BCS}} = 0.8\text{K}$, matching closely with experimental data. Additionally, while a homogeneous (s-wave) gap is obtained, processes for the insulating phases are found to be not described by these effects, a fact observed in previous experimental studies. The simulations are somewhat limited by the truncations used, but nevertheless, a strong candidate for the mechanism behind superconductive phases in twisted bilayer graphene is presented.

Coexisting charge density waves in twisted bilayer NbSe₂

Christopher Tat Shun Cheung - Imperial College London

Twisted moiré bilayers are two-dimensional materials formed by stacking and rotating two monolayer materials. The lattice mismatch generated by such rotation generates a large moiré cell that can contain thousands of atoms, and which can give rise to novel electronic properties. For instance, twisted moiré bilayers of semiconducting transition metal dichalcogenides have been found to host flat electronic bands and correlated electronic phases.

Here we focus on twisted bilayers of metallic NbSe₂. On the one hand, the different local stacking arrangements in the moiré cell cause atomic relaxations (both in-plane and out-of-plane). On the other hand, monolayer NbSe₂ exhibits spontaneous symmetry breaking into a charge density wave state with a 3x3 unit cell lattice reconstruction. In this project we deploy first-principles density functional theory to study and understand the coexistence of these two types of atomic relaxation in twisted NbSe₂ bilayers. We find that different charge density wave states coexist in the ground state of the twisted bilayer: in the low-energy

stacking regions 3x3 charge density waves are found, while stripe charge density waves are found in the domain walls surrounding these regions.

These results demonstrate the possibility to create complex charge density wave ground states in twisted moiré bilayers and can serve as a starting point for predicting superconductivity occurring at low temperatures in these systems.

Best practice around Intel HBM CPUs

Intel / Hewlett Packard Enterprise (HPE)

An update from Intel on the practical usage of the Intel Xeon Max Processor. Specific details around the memory modes, applicability to different types of HPC and AI applications, performance and how to optimize performance when using Max CPU. Following this we will discuss how Intel is implementing memory technology on its latest generation Xeon 6 Processors; providing high memory bandwidth options to the community is critical to support the broad variety of applications within HPC & AI as well as broader markets that are looking to take advantage of additional memory bandwidth to accelerate application performance

Theoretical Investigations on Point Defects in Energy Materials Using a Mott-Littleton Method [Name – University](#)

Cyril Xu - University College London

The presence of point defects in ionic materials determines their ionic conductivity and many other bulk and surface properties, which is central to the discovery of novel materials for energy applications. The n-doped perovskite-structured barium stannate BaSnO₃ is a new generation transparent conducting oxide with excellent prospects in industrial applications. Its ability to sustain high levels of doping while maintaining its crystallinity, transparency, high carrier concentrations and mobility at ambient conditions is related to its defect properties, which are not yet fully understood. Manganese oxide, MnO₂, has been widely recognised as an effective cathode material. Nevertheless, its polymorphic characteristics result in suboptimal performance in industrial applications, prompting the exploration of optimised designs.

Using computer simulations, a variety of material properties can be accurately predicted in a time-efficient manner. An embedded approach, like that developed by Mott and Littleton, is a robust method for the investigation of point defects, based on interatomic potentials.

Employing the Mott-Littleton approach using Norgett's two-region strategy implemented in the General Utility Lattice Programme (GULP), we conducted simulations involving different types of point defects embedded in the perfect BaSnO₃ and ramsdellite-MnO₂ crystal lattices. This approach allows for an accurate and self-consistent description of the effects of the embedding crystal field around the defect and the polarisation. In addition, we used both stochastic and newly-developed exhaustive sampling methods to explore the energy landscape of multiple charged defects. This approach will be demonstrated on both the perovskite and the ramsdellite materials. Our approach is shown to be more efficient than the supercell approach implemented in the periodic ab initio code.

By completing a thorough investigation of the convergence for modelling point defects, we encountered an unexpected behaviour: the defect energy unexpectedly drops periodically after initially showing signs of convergence. Our study revealed a correlation between this behaviour and the unusual anisotropic patterns observed in the defect polarisation field, which differs from patterns seen in simple cubic lattices like MgO. In this talk, I will present both the method developed for this project as well as the data and the analysis of our results.

Identifying CO₂ Conversion Catalysts: High-Throughput DFT Calculations, Machine Learning, and Beyond

Devis Di Tommaso - Queen Mary University of London

The rising carbon dioxide (CO₂) level and overall concentrations in the atmosphere due to fossil fuel combustion, a major cause of global warming, pose a serious threat to humankind.

One of the most promising solutions to mitigating this risk is the chemical conversion of gaseous CO₂ into value-added chemicals and materials. Catalysts can facilitate favourable pathways to reduce the overall energy requirements of the electrochemical CO₂ reduction reaction (eCO₂RR). The eCO₂RR has emerged as a potential strategy for converting CO₂ because if coupled with electricity from renewable sources (wind, solar, or hydropower plants), the eCO₂RR could achieve a carbon-neutral energy cycle [1]. Unfortunately, due to the inertness of CO₂, the main challenge is to find a specific catalyst capable of accelerating the sluggish kinetics of the eCO₂RR. In this talk, I will give an overview of computational strategies we have developed based on the *u* quantum chemical methods [2-4], high-throughput calculations [5], and machine learning [6, 7] methods to accelerate the discovery of earth-abundant and active metal-based catalysts.

References:

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Fast dynamics and high effective dimensionality of liquid and supercritical fluidity Name – University

Cillian Cockrell - Bangor University

Fluidity, the ability of liquids to flow, is the key property distinguishing liquids from solids. This fluidity is set by the mobile transit atoms moving from one quasi-equilibrium point to the next. The nature of this transit motion is unknown.

Here, we use molecular dynamics simulations to show that flow-enabling transits form a dynamically distinct sub-ensemble where atoms move on average faster than the overall system, with a manifestly non-Maxwellian velocity distribution. This is in contrast to solids and gases where no distinction of different ensembles can be made and where the distribution is always Maxwellian. The non-Maxwellian distribution is described by an exponent α corresponding to high dimensionality of space. This is generally similar to extra synthetic dimensions in topological quantum matter, albeit higher dimensionality in liquids is not integer but is fractional. The dimensionality is close to 4 at melting and exceeds 4 at high temperature. α has a maximum as a function of temperature and pressure in liquid and supercritical states, returning to its Maxwell value in the solid and gas states.

Investigating the conductive properties of multi-heme cytochromes

Andras Petho - University College London

Multi-heme cytochromes are fascinating compounds which play a part in the survival of bacteria in anaerobic environments by exporting electrons out of the cells. As such they possess magnitudes larger conductivity compared to non-heme proteins, and thus show exciting potential for constructing biological wires. The reasons behind this increase, despite being observed many times, are unknown.

The goal of this project is to shed light on a possible mechanism of conductivity by looking at how the heme number influences this property. To do this the project will examine proteins with varying number of heme cofactors from one to four, with a possible extension to penta- and hexa-heme proteins. This will be done in tandem with two experimental groups measuring the conductive properties of the proteins in vacuum and in an aqueous environment. Thus, the project will allow a detailed insight into the molecular configurations behind the experimental results. This poster reports the initial results of the project which were acquired from the single-heme MtoD and the tri-heme PpcA.

The results reported here are from the initial junction creation process along with the results of the electronic structure calculations for the gold-protein-gold system. The theory behind acquiring the I-V curves is also introduced. The results show that the process of junction creation using molecular dynamics is reliable, while highlighting the influence of the protein orientation for the conductivity. With the latter causing a magnitude of difference in terms of the simulated current through the junction for a given voltage.

These findings highlight the need for careful consideration when analyzing the results to make the different systems comparable. Nevertheless, the data presented here shows great promise in furthering our understanding of multi-heme cytochromes and their potential for use in the field of bioelectronics.

The (other) big bang theory: towards a structure/property model to rationalise the impact sensitivities of energetic materials

Carole Morrison - University of Edinburgh

Impact sensitivity is a measure of how much mechanical energy is required to initiate explosives and propellants. This important safety metric is typically measured by a simple experiment, where a known weight is dropped from an increasing height, until the minimum threshold energy is observed. However, the data obtained (essentially a binary call of 'go, no-go') is prone to user interpretation and variations in sample purity, crystallinity, temperature, humidity etc. This uncertainty in the experimental measurement has driven the need for physical models that can successfully link the chemical structure to the material property.

Over the last five or so years we have developed a condensed phase model that can link the crystal structure, via its phonon density of states (computed using plane-wave DFT), to its impact sensitivity. Based on the principles of vibrational up-pumping we have now successfully applied this model to ca. 40 energetic materials. However, while it is important for a model to predict the desired property from the given structure, the reverse process is actually more powerful, i.e. for a desired impact sensitivity what sort of molecules should I make? For this more data is needed, and our existing workflow becomes unmanageable. In short, it's time to think about machine learning.

This talk outlines our approach to building a machine learning model for impact sensitivity using features we learned from our vibrational up-pumping model, alongside others that can act to guide synthetic chemists in molecular design. We also consider how to approach the issue of uncertainty in the experimental dataset.

Machine Learning of Polarisation: Problems and Solutions

David Wilkins - Queen's University Belfast

The polarisation of a condensed-phase system, its dipole moment per unit volume, is a key property in predicting the results of vibrational spectroscopy experiments. Although it would seem a natural target for machine-learning methods — and indeed, has been used as one in recent years — doing so comes with some potential problems as the polarisation is not a continuous function of atomic positions.

I will explain how this problem arises, particularly when using pre-existing data, and compare two methods for getting around this problem, both of which allow highly accurate models to be built for polarisation and high-quality predictions to be made for a wide range of vibrational spectra.

Unlocking Conjugated Polymers' Potential: A Data-Driven Approach using PySoftK

Alessandro Santana Bonilla - King's College London

Machine learning methods have revolutionized the design of novel functional materials, but their potential is limited by the scarcity of comprehensive molecular databases.

To address this challenge, we have developed PySoftK, a versatile software package that automates the creation and curation of large polymer libraries with minimal user intervention. By harnessing the power of machine learning, PySoftK enables the efficient generation of complex polymer structures, facilitating the discovery of new materials with novel properties.

In this talk, I present the results of numerical simulations studying the nanoscale structure and emergent optical properties of conjugated polymers like poly(9,9-di-n-octylfluorene-alt-benzothiadiazole) (F8BT), which utilizes PySoftK to model complex polymer structures. The integration of PySoftK with simulation-led design principles provides a predictive understanding by which to enhance the optical properties of next-generation conjugated polymer-based materials, enabling breakthroughs in nanotechnology and biotechnology fields.

Flash Talks

1	Marcus Allen King's College London	A novel 'moment'-based GW algorithm for molecules and solids
2	Wenxuan Cai Imperial College London	Modelling core electron binding energy of metal oxides
3	Dominique de Jong-Hoogland King's College London	Computational Investigation of the Effect of BODIPY Labelling on Peptide-Membrane Interaction
4	Merve Dene University of Reading	Understanding the Hexagonal Boron Nitride / Re (0001) Interface: Experimental and Computational Analysis
5	Basil Ibrahim King's College London	Spectral functions from a Green's function embedding
6	Miguel Luque Canete King's College London	Phonon-limited conductivity of topological surface states in Bi ₂ Se ₃ and graphene
7	Frances Towers Tompkins University of Reading	Anion-Dependent Strength Scale of Interactions in Ionic Liquids: XPS and AIMD
8	Matteo Valderrama Imperial College London	Beyond Graphene: Computational Screening of 2D Materials to Eliminate Friction
9	Chengcheng Xiao Imperial College London	Brillouin zone sampling in ONETEP
10	Chin Yong STFC	D_ATA (Atom Typer and Analyser) – a new software to investigate atomic interactions behaviour

Posters

1	Marcus Allen King's College London	A novel 'moment'-based GW algorithm for molecules and solids
2	Brad Ayers University of Southampton	Atomistic Modelling of Electrified Lithium Anode-Electrolyte Interfaces under Potentiostatic Control
3	Wenxuan Cai Imperial College London	Modelling core electron binding energy of metal oxides
4	Matt Darby Atomic Weapons Establishment	AWE Materials Modelling for Ageing and Lifetime Predictions
5	Dominique de Jong-Hoogland King's College London	Computational Investigation of the Effect of BODIPY Labelling on Peptide-Membrane Interaction
6	Merve Dene University of Reading	Understanding the Hexagonal Boron Nitride / Re (0001) Interface: Experimental and Computational Analysis
7	Basil Ibrahim King's College London	Spectral functions from a Green's function embedding
8	Miguel Luque Canete King's College London	Phonon-limited conductivity of topological surface states in Bi ₂ Se ₃ and graphene
9	Sam Shepherd Queen's University Belfast	Digging into the detail; Discrepancies in the fine structure of kaolin minerals as described by dispersion corrected DFT
10	Christopher Tat Shun Cheung Imperial College London	Coexisting charge density waves in twisted bilayer NbSe ₂
11	Frances Towers Tompkins University of Reading	Anion-Dependent Strength Scale of Interactions in Ionic Liquids: XPS and AIMD
12	Matteo Valderrama Imperial College London	Beyond Graphene: Computational Screening of 2D Materials to Eliminate Friction
13	Ingvars Vitenburgs Imperial College London	Extended Coupled Cluster approach to Twisted Graphene Layers
14	Chengcheng Xiao Imperial College London	Brillouin zone sampling in ONETEP
15	Chin Yong STFC	D_ATA (Atom Typer and Analyser) – a new software to investigate atomic interactions behaviour
16	Ricardo Grau-Crespo Reading	An Experimental and Theoretical Study of Spinel Oxides for Photocatalysis

