Collaborative
Computational Project
Computer Simulation
of Condensed Phases

CCP5 Annual General Meeting

Book of Abstracts

University of Edinburgh

September 9 – 11, 2026

Invited Speakers

Prof Maria Grazia De Angelis
University of Bologna, Italy

Prof Ed Maginn
University of Notre Dame, USA

Prof David Wales
University of Cambridge, UK

Prof Tell Tuttle
University of Strathclyde, UK

Dr James Ewen
University of Bath, UK

Organising Committee

Dr Eleonora Ricci
University of Edinburgh

Prof Clare McCabe
Heriot-Watt University

Dr Claire Hobday
University of Edinburgh

Dr Alin Elena
STFC Daresbury Laboratory

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46th CCP5 Annual General Meeting 2026
Timetable & Programme | 9–11 September 2026
Venue: 2.07 – Yew Lecture Theatre, 2nd Floor, Nucleus Building, Edinburgh

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Dinner: Thu Sep 10, 19:00 Hotel du Vin
Committee: Dr E. Ricci, Prof C. McCabe, Dr C. Hobday, Dr A. Elena
Web: https://agm46.ccp5.ac.uk **Wi-Fi:** Eduroam

September 9, 2026 – Day 1

12:00 – 13:00	LUNCH Arrival, Registration & Lunch
13:00 – 15:00	SESSION 1 **Chair:** Eleonora Ricci
13:00 – 13:15	WELCOME **Prof Chris Lorenz** - CCP5 Chair, King's College London - Welcome and Introduction
13:15 – 14:00	INVITED TALK **Prof David Wales** *(University of Cambridge)* Energy landscapes: Exploration and Discovery
14:00 – 14:20	TALK **Peter Cummings** *(Heriot-Watt University)* Achieving Reproducibility and Replicability of Molecular Dynamics and Monte Carlo Simulations Using the Molecular Simulation Design Framework (MoSDeF)
14:20 – 14:40	TALK **Nasser Afify** *(University of Edinburgh)* Multiscale Atomistic Simulation of Energy Materials and Processes — Limitations and Opportunities
14:40 – 15:00	TALK **Elliott Kasoar** *(STFC/University of Cambridge)* ML-PEG: ML Performance and Extrapolation Guide
15:00 – 15:30	BREAK Coffee Break
15:30 – 16:55	SESSION 2 **Chair:** Alin Elena
15:30 – 16:15	INVITED TALK **Prof Maria Grazia De Angelis** *(University of Bologna)* Bridging AI and Physics-Based Models for Predicting Material Separation Performance
16:15 – 16:35	TALK **Leo Lue** *(University of Strathclyde)* A gradient density functional theory for self-assembling molecular systems
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September 10, 2026 – Day 2 (Morning: Sessions 3 & 4)

09:00 – 10:45	SESSION 3 **Chair:** Andrew Logsdail
09:00 – 09:45	INVITED TALK **Prof Ed Maginn** *(University of Notre Dame)* Thermal Conductivity of Ionic Liquid Mixtures: From Nanostructure to Accurate Molecular Simulation
09:45 – 10:05	TALK **Mazin Saad Almarashi** *(Heriot-Watt University)* Using molecular simulations to examine the interaction of permeation enhancers with the skin barrier
10:05 – 10:25	TALK **Stephen Yeandel** *(University of Bristol)* Computational Insights into Phase Stability and Surface Segregation in GLO
10:25 – 10:45	TALK **Miguel Jorge** *(University of Strathclyde)* Quantifying uncertainty in experimental and simulated adsorption in Metal-Organic Frameworks
10:45 – 11:15	BREAK Coffee Break
11:15 – 12:35	SESSION 4 **Chair:** Clare McCabe
11:15 – 11:35	TALK **Panagiotis Kourtis** *(Newcastle University)* Applications of MACE Foundational Models on Battery Electrolytes
11:35 – 11:55	TALK **Marco Mattia** *(University of Edinburgh)* Learning kinase conformation across activation
11:55 – 12:15	TALK **Sarah Stewart** *(University of Edinburgh)* Amino Acid – Clay Interactions on Mars-Relevant Minerals
12:15 – 12:35	TALK **Stepan Zhikharev** *(University of Warwick)* chirality-kit: A stand-alone topology generator for functionalised and solvated nanostructures.
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13:35 – 14:20	INVITED TALK **Dr James Ewen** *(University of Bath)* Molecular Simulations of Interfacial Processes
14:20 – 14:40	TALK **Michael Seaton** *(UKRI STFC Daresbury Laboratory)* Polarising highly coarse-grained water for aqueous electrolytes
14:40 – 15:00	TALK **Rhys Blaney** *(The University of Strathclyde)* Quantifying Force Field Uncertainty for Biogas Upgrading in Zeolites
15:00 – 15:20	TALK **Asal Azar** *(University of Edinburgh)* Allosteric Regulation of Nitrite Reductase AniA Trimerisation by Copper Binding
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15:50 – 17:30	SESSION 6 **Chair:** Claire Hobday
15:50 – 16:10	TALK **Karen Johnston** *(University of Strathclyde)* A Molecular Dynamics Seeding Approach to Determine Critical Nucleus Size and Concentration for Crystal Nucleation
16:10 – 16:30	TALK **Amro Mohamed** *(Heriot-Watt University)* Computational Screening of Lignin-Derived Epoxy Networks for Gas Separation
16:30 – 16:50	TALK **Jasmine Lightfoot** *(STFC Hartree Centre)* From atoms to application: scalable simulation-driven formulation design
16:50 – 17:10	TALK **Joseph Thomas** *(Northumbria University)* Uncovering Ion Transport Pathways in High-Temperature Green Hydrogen Electrolyser Membranes via Machine-Learned Interatomic Potentials
17:10 – 17:30	TALK **Vanessa Ward** *(Durham University)* Understanding Correlated Motion is Critical to Accurate Predictions of Ionic Conductivity
19:00 – 22:00	DINNER **Conference Dinner** - Hotel du Vin - 11 Bristo Place, Edinburgh, EH1 1EZ

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September 11, 2026 – Day 3 (Sessions 7 & 8)

09:00 – 10:45	SESSION 7 **Chair:** Colin Freeman
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09:45 – 10:05	TALK **Umberto Terranova** *(University of Buckingham)* Iron – Sulfur Cluster Redox Potentials Across Biological Scales
10:05 – 10:25	TALK **Duncan Dockar** *(University of Edinburgh)* Are bulk nanobubbles stabilised by contaminant surfactants?
10:25 – 10:45	TALK **Werner Muller** *(IFP Energies nouvelles)* Developing a Novel Coarse-Grained Force Field for Polyvinyl Chloride: Viscosity Predictions and Uncertainty Quantification
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11:15 – 12:45	SESSION 8 **Chair:** Paola Carbone
11:15 – 11:35	TALK **Andrew Logsdail** *(Cardiff Catalysis Institute, Cardiff University)* Developing new catalysts for CO_2 hydrogenation to fuels through multiscale computational modelling
11:35 – 11:55	TALK **Joseph Burke** *(Imperial College London)* Coarse-grained modelling of porous materials discovery
11:55 – 12:15	TALK **Andreas Hermann** *(The University of Edinburgh)* Atomistic modelling challenges for metal superhydrides
12:15 – 12:35	TALK **Shubham Deshpande** *(Heriot-Watt University)* Investigating the effects of ceramide variation on lipid organisation in the stratum corneum from molecular dynamics simulations
12:35 – 12:45	CLOSING Closing Remarks
12:45 – 14:00	LUNCH Lunch and Departure MEETING *Parallel CCP5 Exec Committee Meeting*

Talks

Multiscale Atomistic Simulation of Energy Materials and Processes — Limitations and Opportunities

Presenter: Nasser Afify
Affiliation: University of Edinburgh

Atomistic simulations have become indispensable tools for understanding and predicting the behaviour of energy materials and processes, providing insights that complement experiments and accelerate the optimisation of engineering systems. Modern atomistic modelling encompasses a broad spectrum of computational methods, ranging from computationally efficient molecular dynamics and Monte Carlo simulations to computationally demanding, high-accuracy first-principles electronic structure calculations. As the target length and time scales increase, however, the direct application of the most accurate methods rapidly becomes computationally prohibitive, necessitating the use of more approximate approaches. A key challenge in multiscale modelling is therefore to combine computationally efficient methods with higher-accuracy electronic structure calculations to achieve predictive simulations while maintaining manageable computational cost. This talk will provide a brief overview of the hierarchy of atomistic simulation methods, highlighting their strengths, limitations, and domains of applicability. It will then showcase recent applications to energy materials and processes, with a particular focus on amine-based post-combustion carbon capture (PCCC) and ammonia-based adsorption refrigeration systems. Emphasis will be placed on selecting the most appropriate computational approach for a given scientific problem and on combining complementary simulation methods to bridge different length and time scales, thereby maximising the insight gained from atomistic simulations. The talk will conclude with a perspective on future directions in multiscale atomistic simulation, including how recent advances in machine learning may help bridge computational methods operating at different levels of accuracy, enabling more predictive simulations of complex energy materials and processes.

Using molecular simulations to examine the interaction of permeation enhancers with the skin barrier

Presenter: Mazin Saad Almarashi
Affiliation: Heriot-Watt University

The stratum corneum (SC), the outermost layer of the skin, acts as an effective barrier to permeation of chemicals both into and out of the skin. Topical drug formulations often include permeation enhancers such as propylene glycol (PG) and isopropanol (IPA) to improve delivery of the active ingredient through the skin barrier. To understand how PEs interact with and influence the structure and organisation of the lipid lamella observed in the SC, molecular dynamics simulations have been conducted to examine the effects of PG and IPA.

Model SC bilayers containing Ceramide Non-hydroxy fatty acid/Sphingosine (Cer[NS]24), lignoceric acid (C24), and cholesterol in a 1:1:0.5 molar ratio have been studied in contact with water containing different concentrations of PG (0–100 weight %) and IPA (0–20 %). PG/water mixtures caused measurable structural changes, including increased area per lipid and reduced bilayer thickness, indicating disruption of lipid packing but limited broadening of the interfacial region. In contrast, IPA was found to have a limited effect on lipid packing but significantly disrupted interfacial order, broadening the interface and increasing lipid mobility.

Solvents containing mixtures of PG and IPA exhibited non-additive effects: the significant interfacial disruption seen with IPA alone was diminished in the presence of PG, while the systems became more structurally heterogeneous. These findings demonstrate that permeation enhancers operate through distinct yet interconnected mechanisms, emphasising how their combined presence modifies bilayer organisation beyond the effects of each component individually. This work adds to a mechanistic framework for understanding enhancer-lipid interactions in the skin barrier.

Allosteric Regulation of Nitrite Reductase AniA Trimerisation by Copper Binding

Presenter: Asal Azar
Affiliation: University of Edinburgh

Metalloenzymes are essential for many biological processes, yet the interplay between metal binding, protein dynamics, and oligomerisation remains poorly understood. We investigate the copper-containing nitrite reductase AniA from Neisseria gonorrhoeae, which exists as a monomer in its apo state and assembles into a catalytically active trimer upon copper loading. As AniA is essential for bacterial survival, understanding its assembly mechanism may provide new strategies to inhibit enzyme function.

A key unresolved question is whether copper binding drives trimerisation or whether trimer formation is required for metal incorporation. To address this, we performed molecular dynamics simulations of apo and holo monomeric and trimeric AniA using quantum-mechanical parameterisation of the copper coordination environment.

Our simulations reveal that the largest structural changes occur in the C-terminal region. This segment is highly flexible in the apo enzyme and remains disordered in the holo monomer but becomes stabilised only in the holo trimer. We further identify an allosteric coupling between the Type-1 and Type-2 copper sites, linking copper binding to trimer assembly. Together, these findings indicate that copper binding alone is insufficient to stabilise the protein, that oligomerisation is required for C-terminal ordering, and that Type-1 copper loading and trimer assembly cooperatively promote formation of the catalytic Type-2 copper site.

Quantifying Force Field Uncertainty for Biogas Upgrading in Zeolites

Presenter: Rhys Blaney
Affiliation: The University of Strathclyde

Rhys Blaney[1], Miguel Jorge[1]

[1]University of Strathclyde, Department of Chemical and Process Engineering, Glasgow, UK

Molecular simulation enables efficient computational screening of porous materials for gas separation, but the reliability of such screening depends on the accuracy of the force field (FF). Previous work from our group quantified FF-selection uncertainty for pure CH_4 and CO_2 adsorption in metal-organic frameworks (MOFs) at 10% [1, 2]. Whether this issue is equally significant for zeolites — a chemically simpler and more industrially established class of porous materials for biogas upgrading (CH_4/CO_2 separation) — remained an open question, with no systematic and rigorous FF evaluation previously carried out for this material group.

This work evaluates twenty FFs — spanning zeolite-specific parametrisations (empirical, semi-empirical, and ab initio), general FFs (e.g. DREIDING, UFF), and FFs developed for other silica-containing systems (e.g. CLAYFF, originally for clay minerals) — for pure CH_4 and CO_2 adsorption in three all-silica zeolites (MFI, DDR, LTA). As individual experimental adsorption measurements can show significant scatter, simulated GCMC isotherms were compared against consensus experimental isotherms — constructed via extensive data mining and statistical analysis following the method of Park et al. [3] — providing both a reliable benchmark for FF performance and an estimate of experimental uncertainty.

Average experimental uncertainties were 8% and 5% for CH_4 and CO_2, respectively — notably lower than the values reported for MOFs, 12% [1] and 14% [2]. However, no FF fell within experimental uncertainty bounds across all studied adsorption systems. The empirical Vlugt FF performed best for CH_4 specifically, while CCFF (derived from dispersion-corrected DFT calculations) showed the most consistent performance across CH_4 and CO_2 and is therefore recommended for screening studies. Both the general FFs and the other silica-derived FFs performed poorly by default, though adapting them to reflect zeolite-specific chemistry (e.g. excluding Si parameters per the Kiselev assumption) improved results.

These results show that FF-selection uncertainty persists even for chemically simpler, well-characterised materials. This has direct implications for the reliability of computational screening results, and quantifying this uncertainty is therefore essential for reporting simulation and screening results with appropriate confidence. This work provides practical guidance on FF choice — and the limits of general and other silica-derived FFs — for computational screening studies.

References

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2C. McCready, K. Asif, R. Blaney, J. Gomes, A. Fletcher, and M. Jorge, Microporous Mesoporous Mater., 2025, 397, 113788-113801.

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Coarse-grained modelling of porous materials discovery

Presenter: Joseph Burke
Affiliation: Imperial College London

New materials are needed to tackle the world's greatest challenges. There are a near-infinite number of synthesisable materials, but we cannot make and test them all. Therefore, predicting the structure and properties of a hypothetical material can narrow the search space which should be explored experimentally, accelerating discovery and increasing efficiency. Established crystal structure prediction techniques have shown excellent accuracy but are highly computationally expensive and scale poorly when screening a large array of molecules, which makes it difficult to elucidate design rules for a system of interest[1].

Our research aims to use coarse-grained (CG) approach gain a better understanding of the interactions which stabilise the crystal structures of porous materials, which can be used to make predictions of their structures. These materials have possible application in gas storage, separation and catalysis so will be vital for making industrial processes more sustainable. CG techniques have been extensively applied to biomolecular systems, where simplification of interactions reduces computational cost, allowing processes to be modelled at longer time and length scales. Following the same logic, we aim to use coarse-graining to simplify the representations of and potentials between molecules and run Monte Carlo (MC) simulations to predict the packing. We hope this will enable large scale screening of possible porous materials such as HOFS and NMOFs.

Thus far, we have modelled T2, successfully reproducing the experimentally determined γ phase [2]. We used a patchy particle model, which has recently been used within the group to predict the packing of the porous organic cages [3], to define hydrogen-bonding interactions. Patches are placed on the hydrogen-bonding components of T2, and the potential energy term is custom made, with a distance dependent and angular dependent term which can be readily tuned to reflect the chemistry of the molecule of interest. Our ambition is to add other intermolecular interaction, such as π-π stacking, to try to reproduce the other polymorphs and apply our modelling method to other porous systems. To this end, we are developing an automated workflow which optimises simulation parameters towards a target using a genetic algorithm. This uses order parameters as a metric to describe each simulation frame, which can inform the algorithm about which parameters to change in the next iteration. We hope to use this approach to explore the phase landscape of different porous systems to identify the key interactions present in experimental structures, which can be used to formulate design rules.

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1.G. J. O. Beran, Chem. Sci., 2023, 14, 13290–13312.

2. A. Pulido, L. Chen, T. Kaczorowski, D. Holden, M. A. Little, S. Y. Chong, B. J. Slater, D. P. McMahon, B. Bonillo, C. J. Stackhouse, A. Stephenson, C. M. Kane, R. Clowes, T. Hasell, A. I. Cooper and G. M. Day, Nature, 2017, 543, 657–664.

3.E. H. Wolpert and K. E. Jelfs, Chem. Sci., 2022, 13, 13588–13599.

A chieving Reproducibility and Replicability of Molecular Dynamics and Monte Carlo Simulations Using the Molecular Simulation Design Framework (MoSDeF)

Presenter: Peter Cummings
Affiliation: Heriot-Watt University

Molecular simulations are increasingly used to predict thermophysical properties and explore molecular-level phenomena beyond modern imaging techniques. To make these tools accessible to nonexperts, several open-source molecular dynamics (MD) and Monte Carlo (MC) codes have been developed. However, using these tools is challenging, and concerns about the validity and reproducibility of the simulation data persist. In 2017, Schappals et al. reported a benchmarking study involving several research groups independently performing MD and MC simulations using different software to predict densities of alkanes using common molecular mechanics force fields [J. Chem. Theory Comput. 2017, 4270-4280]. Although the predicted densities were reasonably close (mostly within 1%), the data often fell outside of the combined statistical uncertainties of the different simulations. Schappals et al. concluded that there are unavoidable errors inherent to molecular simulations once a certain degree of complexity of the system is reached. The Molecular Simulation Design Framework (MoSDeF) is a workflow package designed to achieve TRUE (Transparent, Reproducible, Usable-by-others, and Extensible) simulation studies by standardizing the implementation of molecular models for various simulation engines. This work demonstrates that using MoSDeF to initialize a simulation workflow results in consistent predictions of system density, even while increasing model complexity.

Bridging AI and Physics-Based Models for Predicting Material Separation Performance

Presenter: Maria Grazia De Angelis
Affiliation: University of Bologna

The development of advanced separation materials raises fundamental questions across multiple length scales. How can molecular structure be translated into reliable predictions of sorption, transport, and separation performance? What are the limitations of classical thermodynamic models when applied to emerging materials, from dense polymer membranes for CO capture to porous materials for wearable dialysis? And how can data-driven approaches extend—rather than replace—physically grounded models?

This contribution explores the integration of machine learning with thermodynamic models and molecular simulations. Equation-of-state approaches provide a rigorous framework for describing polymer–penetrant interactions but are often limited by parameter uncertainty and scarce experimental data. Molecular simulations allow prediction of the materials performance from its molecular structure, but they are computationally expensive. Machine learning can help overcome these constraints by incorporating molecular structure directly into thermodynamic models and/or use molecular simulations to train powerful ML models.

The discussion will examine whether machine learning can infer physically meaningful parameters from chemical structure, improve predictions beyond experimentally explored conditions while preserving physical consistency, exploit transfer learning in data-scarce regimes, and allow screening of large material datasets. By combining molecular representations, classical thermodynamics, transport modelling, and data-driven methods, this work aims to advance predictive and interpretable tools for designing materials for CO capture, gas separation, and dialysis.

Investigating the effects of ceramide variation on lipid organisation in the stratum corneum from molecular dynamics simulations

Presenter: Shubham Deshpande
Affiliation: Heriot-Watt University

The stratum corneum (SC) is the outermost layer of human skin and serves as the primary barrier against water loss and external damage. The barrier function of skin arises primarily from the highly ordered lipid matrix between skin (corneocyte) cells. While the composition of the lipid matrix is known, how individual lipids contribute to lipid organisation and barrier function remains poorly understood. Molecular dynamics (MD) simulations can help address this by providing a molecular-level view of skin lipid organisation, allowing the structural roles of individual lipid components to be investigated in model systems.

In this work, MD simulations are used to investigate the structural organisation of SC lipids (ceramides (CERs), cholesterol (CHOL), and free fatty acids (FFAs)) using a multiscale modelling approach. Multilayer lipid systems are first self-assembled using coarse-grained (CG) simulations and subsequently reverse-mapped to atomistic resolution to allow for detailed structural and hydrogen boning analysis. The final atomistic systems consist of six leaflets (three bilayers) and provide a practical representation of the short periodicity phase of the SC. Both pure CER systems and mixtures containing CERs with CHOL and free fatty acids in a 1:0.5:1 molar ratio are examined and metrics such as area per lipid (APL), bilayer height, hydrogen order parameters (SCH), and hydrogen bonding networks are determined. The results demonstrate how slight differences in CER headgroup and tail structure can influence lipid packing and organisation, along with highlighting the capability of the multiscale approach used to complement and explain experimental observations.

Are bulk nanobubbles stabilised by contaminant surfactants?

Presenter: Duncan Dockar
Affiliation: University of Edinburgh

Nanobubbles have been reported to be stable for days to months at a time in experiments, far beyond their ∼1 ms lifetimes expected from classical Epstein-Plesset theory, however, there is no general agreement on the mechanism responsible for this apparent stability. In this work, we use Molecular Dynamics (MD) simulations to investigate a possible stabilisation mechanism where surfactants (which are ubiquitous in nature and engineering, and hence, may be considered practically unavoidable) relax the surface tension of the nanobubble, such that gas pressure decreases with decreasing bubble size, potentially putting the nanobubble in a partially stable mechanical and diffusive equilibrium, which may extend their lifetimes over the classical limits predicted by Epstein-Plesset theory. We extend our modelling using adsorption/desorption rates from the Frumkin adsorption isotherm, to investigate expected lifetimes of typical nanobubbles from the literature and we estimate an upper radius limit of ≤300 nm in which nanobubble lifetimes could be extended by surfactants.

Molecular Simulations of Interfacial Processes

Presenter: James Ewen
Affiliation: University of Bath

Molecular processes at solid-liquid interfaces - such as adsorption and self-assembly of surfactants - are crucial to the macroscale performance of liquid formulations including fuels, lubricants, and cosmetics. In this talk, I will first discuss how molecular simulations at different scales - from density functional theory, to atomistic molecular dynamics (MD), and to coarse grained molecular dynamics - can be used to investigate these process. I will then demonstrate how fundamental insights from MD simulations with enhanced sampling methods can be used to predict experimental adsorption isotherms by utilising molecular thermodynamic theory. Deviations from the standard Langmuir model are discussed and I will propose more advanced alternatives that are motivated from molecular-level insights from the simulations. The improved fundamental understanding of the adsorption process will enable structure-property-performance relationships to be identified for surfactants for formulated products. This will help to accelerate the development of sustainable, high-performance formulations.

Atomistic modelling challenges for metal superhydrides

Presenter: Andreas Hermann
Affiliation: The University of Edinburgh

High-pressure metallic polyhydrides or superhydrides are the best conventional superconductors known, exhibiting transition temperatures close to room temperature, albeit at very high pressures. In principle, due to the electron-phonon coupling mechanism of superconductivity, their electronic and superconducting properties can be determined from first-principles calculations, leading to a large library of predicted compounds. However, discrepancies between such standard ground-state calculations and experiments often arise. Here, we discuss some of the underlying challenges for modelling and how experimental findings can be reconciled with more advanced simulations.

A Molecular Dynamics Seeding Approach to Determine Critical Nucleus Size and Concentration for Crystal Nucleation

Presenter: Karen Johnston
Affiliation: University of Strathclyde

Primary crystal nucleation is dominated by heterogenous pathways, where the crystal nucleus forms at an interface, such as a vessel wall or suspended solid, which affects the nucleation mechanism, rate, and resulting polymorph. Uncertainty remains regarding the nucleation mechanism due to the stochastic nature of the nucleation event which makes experimental observation difficult. In addition, computational methods such as molecular dynamics simulations (MD) are limited due to the computation time required to wait for a rare event to take place. To overcome this, we apply a seeding method using MD to investigate the nucleation of urea. We first consider nucleation in bulk aqueous solutions, before introducing an interface.

Seeding bypasses the need to wait for a rare event to occur. A nanoscale crystal seed is instead simulated in variously concentrated urea solutions, and by observing seed growth and dissolution, we can determine the critical nucleus size and corresponding solution concentration. For critical nuclei with radii ranging from 1.27-4.35 nm, we found that the critical concentration decreased with increasing crystal size (from urea mass fraction 0.95 $\pm$ 0.05 for the smallest critical size to 0.41 $\pm$ 0.02 for the largest critical size). By applying classical nucleation and Ostwald-Freundlich theory, our results showed that the surface energy of nanoscale crystallites is size and concentration dependent. Further investigations into the surface energy dependence on size and solution concentration are needed to provide a better understanding of the nucleation process.

Future work will simulate seed growth and dissolution at an interface, enabling investigation of heterogeneous nucleation. Molecular simulations provide a greater insight into nucleation at a molecular level that will facilitate development of realistic nucleation models and more efficient industrial crystallisation processes.

Quantifying uncertainty in experimental and simulated adsorption in Metal-Organic Frameworks

Presenter: Miguel Jorge
Affiliation: University of Strathclyde

Molecular simulation of adsorption has been shown to be a powerful tool to screen large databases of porous materials (e.g. MOFs) and guide experiments towards the best performing materials. However, comparisons between simulated and experimental adsorption isotherms in MOFs are still fraught with challenges. On the experimental side, there is significant variation between isotherms measured on the same system, with a significant percentage (20%) of published data being considered outliers [1]. On the simulation side, force fields are often chosen "off-the-shelf" with little or no validation. The effect of this choice on the reliability of simulated adsorption predictions has not yet been rigorously quantified. In this work, we fill this gap by systematically quantifying the uncertainty arising from force field selection on adsorption isotherm predictions. We do this by running adsorption simulations with a variety of generic force fields and computing an adsorption "consensus isotherm", including a quantification of parametric uncertainty based on ensemble averaging. This is compared against a similarly generated consensus experimental isotherm constructed from a manually curated set of data from literature. By considering many experimental isotherms measured by different groups and eliminating outliers in the data using statistical analysis, we conduct a rigorous comparison that avoids the pitfalls of the standard approach of comparing simulation predictions to a single experimental isotherm. Our study focuses on methane [2] and carbon dioxide adsorption [3], two of the most relevant greenhouse gases, on a series of prototypical materials that represent the most widely studied MOF "families". Apart from the effect of the framework Lennard-Jones parameters, we also systematically study the effect of point charge assignment (for the polar CO2 molecule) [4], unit cell optimization, cut-off treatment and other relevant simulation parameters. Our results [2-4] show that the uncertainty in simulated isotherms arising from force field selection can be as large as 15%, while the experimental variability can reach 20%, even after outlier removal. We also show that standard "generic" force fields provide unreliable predictions for a large percentage of the systems studied. While most of the discrepancies can be explained by MOF-specific issues (e.g. defects, open metal sites), our observations have profound implications for high-throughput computational screening of MOFs, the reliability of which depends on the accuracy of the underlying force field.

[1] Park, J.; Howe, J. D.; Sholl, D. S., Chemistry of Materials, 29(24), (2017) p. 10487–10495.

[2] McCready, C.; Sladekova, K.; Conroy, S.; Gomes, J. R. B.; Fletcher, A. J.; Jorge, M., J. Chem. Theory Comput., 20, (2024) p. 4869–4884.

[3] McCready, C.; Asif, K.; Blaney, R.; Gomes, J. R. B.; Fletcher, A. J.; Jorge, M., Microporous Mesoporous Mater., 397, (2005) p. 113788.

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[5] Campbell, C.; Gomes, J. R. B.; Fischer, M.; Jorge, M., J. Phys. Chem. Lett., 9, (2018) p. 3544–3553.

ML-PEG: ML Performance and Extrapolation Guide

Presenter: Elliott Kasoar
Affiliation: STFC/University of Cambridge

Recent advances in machine learnt interatomic potentials (MLIPs) are revolutionising atomistic simulations, enabling results with accuracy comparable to ab initio calculations at significantly greater time and length scales. In addition to improved model architectures, access to large, high-quality datasets has enabled the creation of foundational models, trained on sufficiently diverse data to act as a general-purpose model, or starting point, for applications ranging from molecules to proteins. However, as model architectures continue to develop, and new training data becomes available, it has become clear that we are limited in our current methods for rigorously benchmarking foundational MLIPs. Many frequently cited benchmarks are becoming saturated in their scores, focus on a narrow range of systems, such as bulk inorganic crystals, and favour low energy and force errors, rather than more complex physical properties. These limitations inhibit meaningful comparisons of state-of-the-art models, as well as our ability to explain quite diverse performances of models when studying different properties or systems. To address this, we introduce the Machine Learning Performance and Extrapolation Guide (ML-PEG), a hierarchical, customisable, interactive interface, through which the results of benchmarks spanning a wide range of material/molecular applications and physical properties can be examined, ranging from a single numerical score to visualisation of individual atomic structures from a dataset.

Applications of MACE Foundational Models on Battery Electrolytes

Presenter: Panagiotis Kourtis
Affiliation: Newcastle University

Foundational Machine Learned Interatomic Potentials (FMLIPs) have recently emerged as a powerful tool for atomistic simulations. MACE, an equivariant graph neural network potential, is one of the most widely used FMLIP architectures. In this talk I will present applications of MACE FMLIPs to study battery electrolytes. The main questions we aim to answer are:

1.Can out-of-the-box foundational models capture ion diffusion in typical Li-ion carbonate electrolytes?

2.Can long-range, charge-aware models correctly describe redox-active electrolytes such as iron chloride?

3.What is the importance of long-range models for studying concentrated electrolytes such as aqueous ammonium electrolytes?

Weak inter-molecular interactions underpin thermodynamic properties such as the density and diffusivity of a system. We demonstrate the out-of-the-box stability of MACE-MP (one of the early MACE FMLIPs) on a Li PF6, EC/EMC mixture - a common battery electrolyte. Fine-tuning the model with as little as 10 configurations strongly improves the model's inter and intra molecular property predictions. Beyond short-range models, the new charge-aware, MACE-POLAR produces physically relevant partial charges and treats electrostatic interactions across the whole system explicitly via long-range Ewald summation. In an aqueous iron chloride system, this model correctly captures the local reorganization due to different oxidation states of iron. Moreover, we demonstrate that long-range models are important to capture ion-ion correlation effects in concentrated electrolyte systems. We study concentrated aqueous ammonium chloride and ammonium sulphate electrolytes which remain liquid up to high salt concentrations of 6 mol/kg. The OpenFF classical forcefield shows that conductivity including ion-ion correlations estimated using the Green-Kubo formalism converges significantly slower than the typical Nernst-Einstein conductivity. We show that MACE potentials are sufficiently fast to capture nanosecond timescale dynamics at which GK coefficients converge. The remaining question is whether long-range models can correctly predict the experimentally measured ion conductivity.

From atoms to application: scalable simulation-driven formulation design

Presenter: Jasmine Lightfoot
Affiliation: STFC Hartree Centre

As UK industry faces increasing pressure to accelerate innovation while reducing cost and time-to-market, digital technologies are becoming essential components of the R&D process. Computational modelling, high-performance computing, artificial intelligence, and data-driven methodologies enable the rapid exploration of molecular design, chemical formulations, and advanced materials. This de-risks experimental programmes, saving time and resources by identifying high-potential candidates prior to synthesis and manufacture. The STFC Hartree Centre helps translate these cutting-edge computational techniques into industrial impact by developing scalable digital technologies through challenge-led collaborative projects. Through the development, distribution, integration, and training of these digital tools, the Hartree Centre strives to accelerate the adoption of advanced computing across UK industry.

Herein, we outline our pipeline for developing exascale digital solutions to address industrial challenges, showcased through a variety of real-life examples in collaboration with leading UK businesses. We present how lab and manufacturing-scale phenomena can be decomposed into a series of molecular-scale studies. To sample these behaviours, simulation methodologies are developed using quantum (density functional theory), atomistic (all-atom molecular dynamics, grand canonical Monte Carlo), or mesoscopic techniques (coarse-grained molecular dynamics, dissipative particle dynamics), which are built into so-called 'virtual experiments' toolkits. We demonstrate how these simulations techniques and analytical tools have been integrated in custom screening platforms, tailored for deployment within industrial research and development teams. These platforms not only support code democratisation, but also facilitate high-throughput simulation, from which AI and machine learning can be leveraged. In the final stage of our exascale pipeline, we provide examples of how we have paired data-driven approaches with experimental data and simulation techniques to provide at scale molecular screening and predictions. By following this pipeline from end-to-end, we are able to provide scalable and implementable digital methods to tackle industrial challenges, accelerate materials discovery, and guide formulation design.

Developing new catalysts for CO2 hydrogenation to fuels through multiscale computational modelling

Presenter: Andrew Logsdail
Affiliation: Cardiff Catalysis Institute, Cardiff University

Realising a sustainable chemical future requires the development of new catalytic processes. However, the discovery, optimisation, and deployment of catalysts remain challenging, requiring the exploration of vast materials and operating-condition spaces. Experimental screening alone is often costly and time-consuming; consequently, computational modelling now plays a central role in catalyst discovery, focusing experimental effort and establishing an iterative experiment–theory cycle that accelerates mechanistic understanding and guides catalyst design.

In this talk, recent computational studies of heterogeneous catalysts for CO2 hydrogenation to fuels will be presented [1], alongside comparisons with experimental observations [2,3] and examples demonstrating how modelling can inform ongoing catalyst development [4,5]. Emphasis will be placed on our approach to navigating the complex chemical landscape of catalytic materials, combining high-accuracy density functional theory calculations with subgroup discovery (SGD) analysis to identify the key descriptors governing catalytic performance [4,5]. This integrated framework enables both mechanistic insight and predictive catalyst design, revealing how catalyst composition and structure can be tailored to enhance activity, selectivity, and conversion. More broadly, the work illustrates how modern multiscale and data-driven modelling approaches can accelerate the rational development of catalysts for sustainable chemical technologies.

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A gradient density functional theory for self-assembling molecular systems

Presenter: Leo Lue
Affiliation: University of Strathclyde

A novel approximate free energy functional is developed for ideal extended molecular systems, which is applicable to molecules with tree-like architectures and heterogeneous chemistries. In this approach, a non-local functional enforces the chemical bonds between segments within a molecule, which resembles a Coulombic interaction between the bonded segments on the molecules. This ideal functional can be combined with another density functional theory, such as the weighted density approximation, to account for interactions between segments. When combined with a square gradient theory, the resulting approach is a generalization of phenomenological theory developed by Stillinger [FH Stillinger, J. Chem. Phys. 78, 4654 (1983)], which is able to describe the various ordered mesophases, such as the lamellar phase, as well as isotropic micellar aggregates, vesicles, etc. The use of an "Coulomb-like" interaction for bonding was initially recognized by Stillinger and later pursued by other researchers. In this work, the electrostatic analogy is pushed further in this approach, explicitly introducing the "electrostatic potential" into the formulation of the model. This acts as an effective one-body potential required to enforce connectivity within a surfactant molecule; its bulk value plays a role similar to the Donnan potential which is responsible for enforcing bulk electroneutrality. With this formulation, the theory reduces to a set of partial differential equations, rather a set of integral equations. This greatly simplifies the numerical evaluation of the theory, allowing the use of standard finite element or finite volume solvers. This approach enables the simulation of more complex systems and geometries, such as foams. As an example, the formation of stable aggregates, in particular the formation of micelles in aqueous surfactant solutions, is examine through different perspectives, including isodesmic model, density functional theory, integral equation theory, and self-consistent polymer field theories.

Thermal Conductivity of Ionic Liquid Mixtures: From Nanostructure to Accurate Molecular Simulation

Presenter: Edward Maginn
Affiliation: University of Notre Dame

Thermal conductivity (λ) is a critical transport property for the design of separation processes, thermal management systems, and novel fluid materials, yet it remains one of the most challenging properties to predict reliably using molecular dynamics (MD) simulation. This talk presents a coherent account of our recent work on two interconnected problems: understanding the anomalous composition-dependent λ of ionic liquid (IL)/hydrofluorocarbon (HFC) mixtures, and correcting the systematic overestimation of λ that afflicts classical all-atom force fields across virtually all liquid systems.

In the first part of the talk, we combine non-equilibrium MD (NEMD) simulations with transient hot-wire experiments, high-pressure small- and wide-angle X-ray scattering (SAXS/WAXS), electrochemical impedance spectroscopy, and UV-vis solvatochromism to study two mixtures relevant to extractive distillation of refrigerant blends: HFC-134a and HFC-32 dissolved in 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ($[C_2C_1im][TFSI]$). Both systems display anomalous, composition-insensitive λ at low and moderate gas loadings, followed by a sharp decrease at high HFC content. Heat flux decomposition analyses reveal that this behavior is governed by a transition in the dominant molecular mechanism of heat conduction, coinciding with the breakdown of the IL polar network as diagnosed by structure factors computed from MD and measured by X-ray scattering. Ion clustering analyses further show that even after the extended network collapses, ion pairs and small aggregates persist, but the loss of network continuity is sufficient to substantially alter macroscopic heat transport.

The second part of the talk addresses a broader problem: why do classical all-atom force fields systematically overestimate λ for essentially all liquid systems, and what can be done about it? Using heat flux decomposition across a diverse set of molecular liquids, ionic liquids, and IL/HFC mixtures, we identify the overestimation of energy stored and transferred through bonded interactions — particularly high-frequency vibrations involving hydrogen atoms treated classically — as the primary cause. We show that the degree of overestimation scales with molecular size and hydrogen content in a physically interpretable way. Informed by this understanding, we develop a physics-informed algebraic correction model (the HFD-BC method) that, using quantities already computed in the NEMD simulation, corrects raw MD predictions with a mean absolute percentage error below 4% across a broad chemical space that includes molecular liquids, ionic liquids, and complex mixtures — without any re-parameterization of the underlying force field.

Learning kinase conformation across activation

Presenter: Marco Mattia
Affiliation: University of Edinburgh

Kinases are a class of proteins often found overexpressed in cancer cells, making them a candidate for drug design [1]. Several thousand kinase structures have been solved, revealing conserved structure motives that include a disordered region called the ”activation loop” (A-loop). Kinase function is regulated through a conformational switch between an inactive and an active state. Classifying kinase structures in these two conformations can facilitate the selection of promising drug leads [2]. Yet, manual annotation by human experts does not generalise to large-scale studies across the kinome [3]. As more structures become available, our aim is to determine whether there are any structural rearrangement common to all kinase families [4].

We have assembled a dataset comprising of 2523 kinase structures to identify structural patterns that correlate A-loop conformations with kinase activation state. By looking at A-loop conformational states, we automatically annotate kinases into active and inactive states and elucidate their correlation with structural changes across all kinase catalytic domains. We show that classifying conformations based on A-loop geometry yields an 82% accuracy in predicting kinase activation state. Furthermore, a specific distance between the phosphate-binding loop and the C-lobe accounts for the shift in A-loop conformation in 90% of cases. These findings align with previous research on EGFR kinases [5].

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Computational Screening of Lignin-Derived Epoxy Networks for Gas Separation

Presenter: Amro Mohamed
Affiliation: Heriot-Watt University

Lignin-derived aromatic compounds offer a renewable chemical space for the development of epoxy networks for coatings, adhesives and membrane-based gas separations. However, the chemical diversity of lignin conversion streams complicates experimental screening of candidate monomers and formulations. This work presents a multiscale molecular simulation framework for constructing high-conversion lignin-derived epoxy networks and linking monomer chemistry to gas-transport performance.

The workflow uses a hierarchical crosslinking strategy in which network formation is first performed at coarse-grained resolution to accelerate bond formation and enable reproducible screening, followed by back-mapping to atomistic structures for relaxation and property calculation. The resulting networks are characterised in terms of mass density, glass-transition behaviour, free volume, mechanical response, and network connectivity. Gas uptake is evaluated using grand canonical Monte Carlo simulations, while molecular dynamics is used to quantify CO2, N2 and CH4 diffusion and identify the molecular origins of solubility, diffusivity and transport selectivity.

The framework enables three complementary screening routes. First, individual lignin-derived monomers are compared to determine how aromatic structure, functionality and methoxy substitution influence network formation and gas transport. Second, selected monomers are systematically functionalised to enhance CO2-polymer interactions. Third, binary and ternary monomer formulations are studied in an effort to better model realistic lignin-derived feedstocks containing mixtures of depolymerisation products which are then functionalised into epoxy monomers. This methodology links monomer chemistry, functionalisation, composition and curing chemistry to network architecture and gas transport, providing a computational route to build lignin-derived epoxy membranes for CO2/N2 and CO2/CH4 separations.

Developing a Novel Coarse-Grained Force Field for Polyvinyl Chloride: Viscosity Predictions and Uncertainty Quantification

Presenter: Werner Muller
Affiliation: IFP Energies nouvelles

To advance the physical recycling of polyvinyl chloride, a robust molecular understanding of the polymer is essential. Specifically, it is critical to characterise its interactions across a comprehensive dataset of 44 different solvents. In this work, we develop a novel top-down coarse-grained force field to model these polymer-solvent systems efficiently. The predictive capability of this new model is evaluated by comparing it to established coarse-grained force fields, specifically Martini 3 and SAFT-VR. For validation, we also perform reference atomistic simulations utilising the OPLS force field. Our investigation focuses on calculating key thermodynamic, structural, and transport properties, specifically solubility parameters, the radius of gyration, and self-diffusion coefficients. A central aspect of this study is the direct comparison of calculated polymer viscosity with experimental results across these varied solvent environments. Finally, to ensure the reliability of our computational data, we investigate uncertainty quantification by evaluating statistical variance across multiple simulation replicas.

Polarising highly coarse-grained water for aqueous electrolytes

Presenter: Michael Seaton
Affiliation: UKRI STFC Daresbury Laboratory

When simulating polar solvents at larger-than-atomistic (e.g. mesoscopic) length and time scales, the primary challenge is to devise suitable interaction models. These should not only produce realistic thermodynamic and hydrodynamic behaviours, but also incorporate polar behaviours such as correct bulk relative permittivities and dielectric responses to interfaces and electric fields generated by ionic species.

Considering the most abundant polar solvent – water – we propose a number of interaction models that attempt to produce correct properties across the board for a large coarse-graining (CG) degree of 5 molecules per calculation entity. Starting with pairwise particle interactions modified from those typically used in Dissipative Particle Dynamics (DPD) to produce more realistic thermodynamic behaviours, we attached Drude smeared charges to generate additional dipole moments. After deciding which particles in our CG water entity hold charges and their magnitudes, we devised three polar water models based on varying the flexibility of bond interactions between central interacting particles and Drude charges: all three were parameterised to obtain the correct relative permittivity for water at room temperature. We also propose the use of the pairwise DPD thermostat to tune hydrodynamically relevant properties.

As well as examining measurable physical properties for these water models, including interfacial tension, self-diffusivity and shear viscosity, we examined the generated dipole and quadrupole moment distributions as well as their responses to external electric fields. We compared these with distributions obtained by systematically coarse-graining a molecular dynamics trajectory of a popular atomistic water model (TIP3P), either by clustering together intact water molecules or by bringing together the nearest stoichiometrically-correct atoms without considering molecular topology. This exercise also enabled us to determine the best-suited CG levels for water, justifying our choice of 5:1 and the use of flexible bonds to attach charges to central interacting beads.

Finally, we outline how we applied our polarisable 5:1 CG water model to model the water-based electrolytes found in vanadium redox flow batteries (VRFB). This included selecting how ionic species are represented in the catholyte and anolyte – making use of the original non-polar CG water model – and how the DPD thermostat was parameterised to obtain their correct diffusivities.

PolyRapid: Automated High-Throughput Screening of Polymers Using a Computational Workflow

Presenter: Lois Smith
Affiliation: University of Liverpool

High-throughput computational screening of polymers offers a powerful way to address the imbalance between the vast number of polymers synthesised for diverse applications and the relatively small subset that can be studied using atomistic simulations. This work presents PolyRapid: an automatic workflow designed to enable the rapid and efficient screening of an extensive polymer library. In this work it is deployed on a library of 103 homopolymers. The workflow integrates an automated annealing protocol with adaptive control, allowing for reproducible simulations with minimal human intervention and minimisation of the computational cost. It achieves equilibration in 95% of systems within four 30 ns annealing cycles, and 100% within 9 annealing cycles. The availability of a homogenous large set of simulations enables the adoption of machine learning approaches for a variety of tasks. We exemplify this possibility by proposing rapid machine-learning-based method to predict the (computed) polymer density (F1-score = 0.91) and (experimental) glass transition temperature (F1-score = 0.76), using both chemical fingerprint representations and physically meaningful MD-derived descriptors.

Amino Acid–Clay Interactions on Mars-Relevant Minerals

Presenter: Sarah Stewart
Affiliation: University of Edinburgh

Clay minerals have a track record of long-term preservation of organics, making clay-rich soils of interest to Martian missions.[1] Amino acids are among the building blocks of life, easily synthesised, and commonly found in space.[2] However, their ubiquity means that, even preserved on extraterrestrial rocky bodies, amino acids alone do not constitute a biosignature. Clay minerals are not only capable of adsorbing amino acids, but also polymerizing them into a peptide,[3] which makes the identification of a true biosignature even more difficult.

In this case, one must find routes to distinguish these pseudo-biosignatures from true ones, that would have emerged and functioned elsewhere and only later preserved by the clay. In view of sample return missions, one must find a route to discard the samples containing pseudo-biosignatures.[4] Ideally, we must do so by only knowing the retained amino acid distribution and the mineral structure, as this is the data we realistically could obtain.[5]

To this end, we have studied the adsorption of 20 proteinogenic L-amino acids onto four Mars-relevant clays: montmorillonite (SWy1), beidellite (SBCa1), ferruginous smectite (SWa1) and saponite (SapCa2). The effect of mineral composition and counterions (Na+, K+, Mg2+ or Ca2+) on adsorption was quantified and compared. The knowledge of the selectivity of the mineral toward adsorbed species allows us to suggest the composition of a polymer generated by this mineral surface. Anything matching the predicted composition can be confidently discarded as a pseudo-biosignature. On the other hand, the presence of amino acids that are unlikely to be adsorbed by this mineral under the given conditions will suggest the sample should be investigated further and potentially returned to Earth for in-depth studies.[4]

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Iron–Sulfur Cluster Redox Potentials Across Biological Scales

Presenter: Umberto Terranova
Affiliation: University of Buckingham

Iron–sulfur (FeS) clusters are central to biological electron transfer. Understanding

their redox properties is essential for elucidating their role in both natural and

bioinspired systems. Here, I present QM/MM calculations under the linear response

approximation of FeS clusters redox potentials in two distinct biological contexts: (i) ferredoxin-maquette peptides at the interface with hydrogenase and (ii) the SARS-CoV-2 replication and transcription complex (RTC) that governs the viral life cycle. In the first case, I will show that the redox potential of the peptides can be fine-tuned by single-residue mutations in the secondary coordination sphere of their FeS cluster. In particular, I have designed a variant of a canonical peptide that disrupts the hydrogen-bonding network between the cluster and water, causing a negative redox potential shift of 0.03 V [1]. In the second case, I will examine the four FeS cofactors of two essential proteins of the SARS-CoV-2 RTC [2]. The redox potentials of these clusters fall within the range –0.26 to 0.04 V, following a trend consistent with their measured electronegativities [3]. Together, these studies demonstrate the applicability of QM/MM methods based on the linear response approximation to a variety of FeS systems ranging from small peptides to large multiprotein assemblies.

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Uncovering Ion Transport Pathways in High-Temperature Green Hydrogen Electrolyser Membranes via Machine-Learned Interatomic Potentials

Presenter: Joseph Thomas
Affiliation: Northumbria University

With the transition to net zero, scalable methods for converting renewable electricity into storable energy carriers are essential. Green hydrogen is a promising energy carrier that can store intermittent renewable electricity and serve as a replacement for natural gas in hard-to-decarbonise industries. Proton exchange membrane water electrolysers (PEMWEs) are particularly attractive for green hydrogen production due to their technological maturity, high hydrogen purity, compact design, and fast dynamic response compared to other commercially available water electrolysers [1].

A major barrier to PEMWE commercialisation is the reliance on scarce noble metal catalysts, particularly iridium. Operating at elevated temperatures (100–200 °C) enhances electrochemical kinetics, potentially enabling reduced iridium loadings and lower system costs. However, conventional Nafion membranes degrade above 125 °C [2], necessitating thermally stable alternatives. Polybenzimidazole (PBI) membranes are promising candidates due to their exceptional thermal stability and proton conductivity when acid-doped, with operational capability in the 100–200 °C regime [3]. Nevertheless, PBI's lower ionic conductivity compared to Nafion remains a performance bottleneck. Elucidating proton transport mechanisms in PBI at the molecular level is therefore critical for designing improved high-temperature membranes that can enable cost-effective, large-scale green hydrogen production.

Atomistic simulations face a fundamental challenge in this context: classical molecular dynamics cannot capture proton hopping, while density functional theory (DFT)-based molecular dynamics is restricted to system sizes too small to be physically representative. Machine-learned interatomic potentials overcome this limitation by retaining near-DFT accuracy at approximately two orders of magnitude lower computational cost [4]. Here, we show that the MACE foundational model accurately reproduces first-principles molecular dynamics for acid-doped PBI systems, despite being trained exclusively on crystalline materials rather than polymeric systems, demonstrating strong transferability and generalisation of the machine-learned interatomic potential. This validation enables large-scale simulations with explicit proton dynamics, revealing a previously unrecognised water-mediated proton transfer pathway that provides new design principles for high-performance membranes enabling low-cost green hydrogen production.

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Peptides at the Edge: Designing Function at Mineral and Ice Interfaces

Presenter: Tell Tuttle
Affiliation: University of Strathclyde

Peptides provide a versatile platform for designing functional materials, combining chemical programmability with the ability to assemble, bind, and adapt at complex interfaces. Using molecular simulation, machine learning, and structure prediction, we explore how sequence encodes material function across systems ranging from enamel-inspired biomolecular assemblies to antifreeze peptides interacting with ice–water interfaces. These studies highlight both the challenges and opportunities in designing peptides as active mediators of interfacial organisation, and point toward broader principles for engineering function at highly structured interfaces, from biological minerals to frozen water.

Energy landscapes: Exploration and Discovery

Presenter: David Wales
Affiliation: University of Cambridge

The potential energy landscape provides a conceptual and computational framework for investigating structure, dynamics, and thermodynamics in atomic and molecular science.

This talk will present recent developments for global optimisation, quantum dynamics, thermodynamic properties of systems exhibiting broken ergodicity, and associated rare event dynamics,

with applications to biophysics, self-organisation, and tunneling phenomena.

Theory developed for molecular systems can be used to analyse the solution space for applications to machine learning, self-consistent fields, and quantum computing.

Single funnel landscapes encode efficient self-organisation, explaining how the Levinthal Paradox can be overcome in proteins and in general.

In contrast, multifunnel landscapes exhibit characteristic features in thermodynamic observables, such as the heat capacity, and multiple relaxation time scales in first passage time distributions.

For example, a molecular switch corresponds to a double funnel landscape, while multifunnel landscapes underpin multifunctional capabilities of biomolecules.

Understanding how to tune the landscape from self-organising to glassy properties represents a key design principle for systems with target emergent properties.

Selected Publications:

Nat. Commun (2024) 15, 8763. Design principles for energy transfer in the photosystem II supercomplex.

npj Quantum Information, 9, 75, 2023. Exact Electronic States With Shallow Quantum Circuits From Global Optimisation

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Understanding Correlated Motion is Critical to Accurate Predictions of Ionic Conductivity

Presenter: Vanessa Ward
Affiliation: Durham University

A comprehensive understanding of ion transport is necessary for predicting conductivity in solid electrolytes. It is also key to the rational design of new materials. Ion transport is a dynamic process spanning a wide range of timescales, from the atomic level to the device scale. Here, we focus on how transport mechanisms at an atomistic level affect macroscopic transport coefficients.

There are a number of different ways in which motion can be correlated. It is possible to derive a mathematical framework for the correlations in both liquids and solids. Firstly, the motion of an individual ion may not follow a random walk and there is self correlation. Self-correlated events include an ion returning to a previous position, in a back-and-forth motion. Ions may become trapped due to local structure, particularly if there are limited directions of travel available. They

will undergo significant movement, but in a back-and-forth motion that does not contribute to overall transport.

In contrast, distinct correlations involve multiple ions. For example, one ion may vacate a position and the newly created vacancy allows another ion to move. These moves could occur concurrently or sequentially. It is also worth noting that moves that appear connected may actually be dynamically independent, occurring only as a consequence of the structural change caused by a previous event. An induced rather than a synchronous collective mechanism. We compare different methods for identifying distinct correlations including k-means clustering and directed graphs. Characterising these correlations is an important step in the design of next-generation batteries.

Computational Insights into Phase Stability and Surface Segregation in GLO

Presenter: Stephen Yeandel
Affiliation: University of Bristol

Europium-doped (GdxLu1-x)2O3 (GLO) is a promising scintillator material, offering high transparency and strong luminescence for next-generation applications. Optimising GLO for efficiency, crystal quality and manufacturability requires a clear understanding of the thermodynamic stability and the factors governing dopant distribution.

In this work, we employ atomistic modelling to quantify the mixing behaviour of the Gd2O3 – Lu2O3 solid solution. Using hybrid Molecular Dynamics/Monte-Carlo simulations, we have determined the relative chemical potential ($\Delta\mu$_Lu/Gd) as a function of stoichiometry and temperature. Fitting our results to an asymmetric Margules model has yielded the GLO phase diagram and indicates a critical miscibility temperature of 670 K.

Furthermore, our simulations have revealed significant surface enrichment of Gd ions. This segregation will have a strong influence on the evolution of grain boundaries during sintering and will directly impact the final quality of GLO crystals.

chirality-kit: A stand-alone topology generator for functionalised and solvated nanostructures.

Presenter: Stepan Zhikharev
Affiliation: University of Warwick

Single-walled carbon nanotubes (CNTs) show promise for efficient and tunable ionic transport through the alteration of their surface chemistry. Tunable permselective properties can be achieved by precisely combining functional groups, and general trends can be observed through a comprehensive study of CNT and functional-group configuration space. However, it is currently challenging to generate bespoke topologies of functionalised carbon nanotubes, especially in classical force fields, where each bonded coefficient has to be explicitly written to the relevant topology file. Numerical integrators for classical force fields also require significant attention, as without charge neutrality, the Ewald summation does not converge correctly, and hence the electrostatic non-bonded interactions are not reflective of the force field. To address these challenges of streamlining the process of nanochannel setup, chirality-kit was created. The repository was natively built for classical force fields, providing consistency in topology creation, allowing charge minimisation through ion injection as well as charge adjustment through perturbation of charge of virtual ion sites. This native support also extends to the explicitly polarisable Drude-particle force fields. Comprehensive support for solvent and ion injection, including geometry-aware concentration targeting and minimum-distance placement exists for any well defined molecule topology and can be used independently of nanochannel creation. Although designed around classical force-field workflows, chirality-kit also supports the generation of structures for machine-learned interatomic potentials, enabling the same construction, functionalisation, and solvation tools to be used in topology-free simulation workflows. This project is in active development with support already available for carbon, copper, boron-nitride, MoS2, and MoSSe nanotubes.

Posters

Using molecular simulations to examine the interaction of permeation enhancers with the skin barrier

Presenter: Mazin Saad Almarashi
Affiliation: Heriot-Watt University

The stratum corneum (SC), the outermost layer of the skin, acts as an effective barrier to permeation of chemicals both into and out of the skin. Topical drug formulations often include permeation enhancers such as propylene glycol (PG) and isopropanol (IPA) to improve delivery of the active ingredient through the skin barrier. To understand how PEs interact with and influence the structure and organisation of the lipid lamella observed in the SC, molecular dynamics simulations have been conducted to examine the effects of PG and IPA.

Model SC bilayers containing Ceramide Non-hydroxy fatty acid/Sphingosine (Cer[NS]24), lignoceric acid (C24), and cholesterol in a 1:1:0.5 molar ratio have been studied in contact with water containing different concentrations of PG (0–100 weight %) and IPA (0–20 %). PG/water mixtures caused measurable structural changes, including increased area per lipid and reduced bilayer thickness, indicating disruption of lipid packing but limited broadening of the interfacial region. In contrast, IPA was found to have a limited effect on lipid packing but significantly disrupted interfacial order, broadening the interface and increasing lipid mobility.

Solvents containing mixtures of PG and IPA exhibited non-additive effects: the significant interfacial disruption seen with IPA alone was diminished in the presence of PG, while the systems became more structurally heterogeneous. These findings demonstrate that permeation enhancers operate through distinct yet interconnected mechanisms, emphasising how their combined presence modifies bilayer organisation beyond the effects of each component individually. This work adds to a mechanistic framework for understanding enhancer-lipid interactions in the skin barrier.

Allosteric Regulation of Nitrite Reductase AniA Trimerisation by Copper Binding

Presenter: Asal Azar
Affiliation: University of Edinburgh

Metalloenzymes are essential for many biological processes, yet the interplay between metal binding, protein dynamics, and oligomerisation remains poorly understood. We investigate the copper-containing nitrite reductase AniA from Neisseria gonorrhoeae, which exists as a monomer in its apo state and assembles into a catalytically active trimer upon copper loading. As AniA is essential for bacterial survival, understanding its assembly mechanism may provide new strategies to inhibit enzyme function.

A key unresolved question is whether copper binding drives trimerisation or whether trimer formation is required for metal incorporation. To address this, we performed molecular dynamics simulations of apo and holo monomeric and trimeric AniA using quantum-mechanical parameterisation of the copper coordination environment.

Our simulations reveal that the largest structural changes occur in the C-terminal region. This segment is highly flexible in the apo enzyme and remains disordered in the holo monomer but becomes stabilised only in the holo trimer. We further identify an allosteric coupling between the Type-1 and Type-2 copper sites, linking copper binding to trimer assembly. Together, these findings indicate that copper binding alone is insufficient to stabilise the protein, that oligomerisation is required for C-terminal ordering, and that Type-1 copper loading and trimer assembly cooperatively promote formation of the catalytic Type-2 copper site.

Coarse-grained modelling of porous materials discovery

Presenter: Joseph Burke
Affiliation: Imperial College London

New materials are needed to tackle the world's greatest challenges. There are a near-infinite number of synthesisable materials, but we cannot make and test them all. Therefore, predicting the structure and properties of a hypothetical material can narrow the search space which should be explored experimentally, accelerating discovery and increasing efficiency. Established crystal structure prediction techniques have shown excellent accuracy but are highly computationally expensive and scale poorly when screening a large array of molecules, which makes it difficult to elucidate design rules for a system of interest[1].

Our research aims to use coarse-grained (CG) approach gain a better understanding of the interactions which stabilise the crystal structures of porous materials, which can be used to make predictions of their structures. These materials have possible application in gas storage, separation and catalysis so will be vital for making industrial processes more sustainable. CG techniques have been extensively applied to biomolecular systems, where simplification of interactions reduces computational cost, allowing processes to be modelled at longer time and length scales. Following the same logic, we aim to use coarse-graining to simplify the representations of and potentials between molecules and run Monte Carlo (MC) simulations to predict the packing. We hope this will enable large scale screening of possible porous materials such as HOFS and NMOFs.

Thus far, we have modelled T2, successfully reproducing the experimentally determined γ phase [2]. We used a patchy particle model, which has recently been used within the group to predict the packing of the porous organic cages [3], to define hydrogen-bonding interactions. Patches are placed on the hydrogen-bonding components of T2, and the potential energy term is custom made, with a distance dependent and angular dependent term which can be readily tuned to reflect the chemistry of the molecule of interest. Our ambition is to add other intermolecular interaction, such as π-π stacking, to try to reproduce the other polymorphs and apply our modelling method to other porous systems. To this end, we are developing an automated workflow which optimises simulation parameters towards a target using a genetic algorithm. This uses order parameters as a metric to describe each simulation frame, which can inform the algorithm about which parameters to change in the next iteration. We hope to use this approach to explore the phase landscape of different porous systems to identify the key interactions present in experimental structures, which can be used to formulate design rules.

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Investigating the effects of ceramide variation on lipid organisation in the stratum corneum from molecular dynamics simulations

Presenter: Shubham Deshpande
Affiliation: Heriot-Watt University

The stratum corneum (SC) is the outermost layer of human skin and serves as the primary barrier against water loss and external damage. The barrier function of skin arises primarily from the highly ordered lipid matrix between skin (corneocyte) cells. While the composition of the lipid matrix is known, how individual lipids contribute to lipid organisation and barrier function remains poorly understood. Molecular dynamics (MD) simulations can help address this by providing a molecular-level view of skin lipid organisation, allowing the structural roles of individual lipid components to be investigated in model systems.

In this work, MD simulations are used to investigate the structural organisation of SC lipids (ceramides (CERs), cholesterol (CHOL), and free fatty acids (FFAs)) using a multiscale modelling approach. Multilayer lipid systems are first self-assembled using coarse-grained (CG) simulations and subsequently reverse-mapped to atomistic resolution to allow for detailed structural and hydrogen boning analysis. The final atomistic systems consist of six leaflets (three bilayers) and provide a practical representation of the short periodicity phase of the SC. Both pure CER systems and mixtures containing CERs with CHOL and free fatty acids in a 1:0.5:1 molar ratio are examined and metrics such as area per lipid (APL), bilayer height, hydrogen order parameters (SCH), and hydrogen bonding networks are determined. The results demonstrate how slight differences in CER headgroup and tail structure can influence lipid packing and organisation, along with highlighting the capability of the multiscale approach used to complement and explain experimental observations.

Hydrogen bonds at high pressure: symmetrisation and beyond

Presenter: Andreas Hermann
Affiliation: The University of Edinburgh

Hydrogen bonds are crucial for the structure of water, protein folding, the DNA helix, and inorganic and mineral compounds. They are roughly an order of magnitude stronger than dispersion interactions, and an order of magnitude weaker than covalent bonds, and therefore very susceptible to pressure changes in the 1-100 GPa pressure range, where they can drive changes to local structure, densities, and elastic properties. At high temperatures, the presence of hydrogen bonds influences proton mobility and therefore ionic conductivities. Here, I will give an overview of some of our recent computational work, where we have studied the pressure dependence of hydrogen bonds in planetary ices, hydrous minerals, and other inorganic compounds. I will focus especially on the phenomenon of hydrogen bond symmetrisation, where protons sit at the mid-point between two anions, and which in many systems marks a pressure-induced transition from bonded molecular or cluster compounds to atomic framework compounds, with consequences for spectroscopic, elastic, and transport properties.

Applications of MACE Foundational Models on Battery Electrolytes

Presenter: Panagiotis Kourtis
Affiliation: Newcastle University

Foundational Machine Learned Interatomic Potentials (FMLIPs) have recently emerged as a powerful tool for atomistic simulations. MACE, an equivariant graph neural network potential, is one of the most widely used FMLIP architectures. In this talk I will present applications of MACE FMLIPs to study battery electrolytes. The main questions we aim to answer are:

1.Can out-of-the-box foundational models capture ion diffusion in typical Li-ion carbonate electrolytes?

2.Can long-range, charge-aware models correctly describe redox-active electrolytes such as iron chloride?

3.What is the importance of long-range models for studying concentrated electrolytes such as aqueous ammonium electrolytes?

Weak inter-molecular interactions underpin thermodynamic properties such as the density and diffusivity of a system. We demonstrate the out-of-the-box stability of MACE-MP (one of the early MACE FMLIPs) on a Li PF6, EC/EMC mixture - a common battery electrolyte. Fine-tuning the model with as little as 10 configurations strongly improves the model's inter and intra molecular property predictions. Beyond short-range models, the new charge-aware, MACE-POLAR produces physically relevant partial charges and treats electrostatic interactions across the whole system explicitly via long-range Ewald summation. In an aqueous iron chloride system, this model correctly captures the local reorganization due to different oxidation states of iron. Moreover, we demonstrate that long-range models are important to capture ion-ion correlation effects in concentrated electrolyte systems. We study concentrated aqueous ammonium chloride and ammonium sulphate electrolytes which remain liquid up to high salt concentrations of 6 mol/kg. The OpenFF classical forcefield shows that conductivity including ion-ion correlations estimated using the Green-Kubo formalism converges significantly slower than the typical Nernst-Einstein conductivity. We show that MACE potentials are sufficiently fast to capture nanosecond timescale dynamics at which GK coefficients converge. The remaining question is whether long-range models can correctly predict the experimentally measured ion conductivity.

Developing a Novel Coarse-Grained Force Field for Polyvinyl Chloride: Viscosity Predictions and Uncertainty Quantification

Presenter: Werner Muller
Affiliation: IFP Energies nouvelles

To advance the physical recycling of polyvinyl chloride, a robust molecular understanding of the polymer is essential. Specifically, it is critical to characterise its interactions across a comprehensive dataset of 44 different solvents. In this work, we develop a novel top-down coarse-grained force field to model these polymer-solvent systems efficiently. The predictive capability of this new model is evaluated by comparing it to established coarse-grained force fields, specifically Martini 3 and SAFT-VR. For validation, we also perform reference atomistic simulations utilising the OPLS force field. Our investigation focuses on calculating key thermodynamic, structural, and transport properties, specifically solubility parameters, the radius of gyration, and self-diffusion coefficients. A central aspect of this study is the direct comparison of calculated polymer viscosity with experimental results across these varied solvent environments. Finally, to ensure the reliability of our computational data, we investigate uncertainty quantification by evaluating statistical variance across multiple simulation replicas.

chirality-kit: A stand-alone topology generator for functionalised and solvated nanostructures.

Presenter: Stepan Zhikharev
Affiliation: University of Warwick

Single-walled carbon nanotubes (CNTs) show promise for efficient and tunable ionic transport through the alteration of their surface chemistry. Tunable permselective properties can be achieved by precisely combining functional groups, and general trends can be observed through a comprehensive study of CNT and functional-group configuration space. However, it is currently challenging to generate bespoke topologies of functionalised carbon nanotubes, especially in classical force fields, where each bonded coefficient has to be explicitly written to the relevant topology file. Numerical integrators for classical force fields also require significant attention, as without charge neutrality, the Ewald summation does not converge correctly, and hence the electrostatic non-bonded interactions are not reflective of the force field. To address these challenges of streamlining the process of nanochannel setup, chirality-kit was created. The repository was natively built for classical force fields, providing consistency in topology creation, allowing charge minimisation through ion injection as well as charge adjustment through perturbation of charge of virtual ion sites. This native support also extends to the explicitly polarisable Drude-particle force fields. Comprehensive support for solvent and ion injection, including geometry-aware concentration targeting and minimum-distance placement exists for any well defined molecule topology and can be used independently of nanochannel creation. Although designed around classical force-field workflows, chirality-kit also supports the generation of structures for machine-learned interatomic potentials, enabling the same construction, functionalisation, and solvation tools to be used in topology-free simulation workflows. This project is in active development with support already available for carbon, copper, boron-nitride, MoS2, and MoSSe nanotubes.

Molecular modelling of anion-exchange membranes

Presenter: Khaled Almulafekh
Affiliation: University of Edinburgh - Institute of Materials and Processes

The transition to a net-zero energy system depends on clean-energy conversion devices, with fuel cells central to the hydrogen economy.1 Proton-exchange membrane fuel cells are well established but costly, relying on platinum catalysts and fluorinated polymers.2 Anion-exchange membrane fuel cells (AEMFCs) offer an economical alternative, since alkaline operation permits the use of abundant, non-precious-metal catalysts.2 Their viability is held back by a coupled trade-off: a single membrane must combine chemical stability, mechanical strength, and ionic conductivity, and gains in one property are often offset by losses in another.2 Rational design of durable, conductive anion-exchange membranes (AEMs) therefore calls for predictive insight at the molecular scale.

This work develops validated molecular-simulation protocols targeting these three properties as a function of hydration, using Sustainion as a representative AEM. Dry equilibration by equilibrium molecular dynamics (MD) first validates force-field selection against the dry-state density across three independent replicas. The SciPCFF force field reproduced a consistent dry-state density, agreeing with the experimental value to within 2%. Mechanical strength is assessed by uniaxial tensile deformation at four strain rates, with the Young's modulus extracted through an automated pipeline devised for the extraction of statistically significant metrics from noisy data series, taking into account temporal correlation. The pipeline returned a Young's modulus on the order of 3 GPa across different strain rates. For hydration-dependent transport, iterative grand-canonical Monte Carlo coupled to MD (GCMC-MD) produced non-convergent water uptake. Therefore, continuous fractional-component Monte Carlo (CFCMC) simulations were implemented for equilibrium water sorption. Chemical stability was examined with density functional theory (DFT) to obtain the activation barriers and reaction free energies of candidate degradation pathways such as SN2 substitution and Hofmann elimination at the cationic head groups, drawing on established quantum-chemical approaches.

Together, these establish a reproducible framework linking molecular interactions to the chemical, mechanical, and transport properties behind the AEM trade-off.

Keywords: anion-exchange membrane; molecular dynamics; chemical stability; mechanical properties; ionic conductivity

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Towards Optimization of Coarse-Grained Forcefields for Polymers Using Gaussian Processes

Presenter: Miltiades Angelides
Affiliation: University of Manchester

Polymer simulation properties can be highly sensitive to long-range interatomic interactions and are thus of critical importance to capture correctly when parameterizing forcefields. In this work, Gaussian Process guided Molecular Dynamics simulations are used to parameterize coarse-grained forcefields of polymers targeting emergent bulk behaviours. A Gaussian Process is trained as a surrogate model predicting entanglement length from selected forcefield parameters which are then used to initiate simulations expected to reproduce target behaviours. An automated workflow enables the iterative improvement of the model through repeated training using goal-oriented simulation parameters. This approach allows for the efficient parameterization of coarse-grained forcefields for polymer molecular dynamics.

Evaluating ML Performance on Actinide Oxide Systems

Presenter: Daniel Brown
Affiliation: University of Huddersfield

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Actinide oxides (UO2, PuO2, ThO2) are central to the nuclear fuel cycle. Furthermore, their lanthanide analogues such as CeO2 are often used as simulant materials because they are not radioactive. Modelling of these materials is a route often used to study them however their complex f-electron behaviour makes accurate, large-scale simulation of their lattice behaviour challenging. Machine learned interatomic potential (MLIPs) are an emergent technology that offer near-density-functional-theory (DFT) accuracy at a speed more comparable to classical potentials. This allows for far larger simulation length and time scales of these materials to be explored.

This work evaluates the MACE-MH-1 foundational model against experimental data for the lattice parameters for all four AnO2 across 300-3000K, finding good agreement at low temperatures but showing a progressive loss of accuracy at higher temperatures. Molecular dynamics trajectories generated with MACE-MH-1 were then used to select representative CeO2 configurations. Farthest-point sampling and SOAP descriptors were used to ensure the diversity of the energy landscape was captured for the full temperature range. Using these configurations, reference energies, forces, and stress were computed via DFT single-point calculations to yield a training set that was used to fine tune the foundational model. The fine tuned model was then benchmarked against the foundational model and experimental data.

Understanding Gas Transport at a Polymer/MOF Interface through Molecular Modelling Techniques

Presenter: Tiziano Cavalieri
Affiliation: The University of Edinburgh

Mixed Matrix Membranes (MMMs) are emerging composite materials made of nanoparticles dispersed in a polymeric matrix. In the recent years they are gaining increasing attention in gas separation processes due to the possibility to outperform dense polymeric membranes thanks to the improved performance arising from the combination of suitable matrix and filler. However, the interactions between the two class of materials, particularly at the interface, are complex and non-ideal. A complete theoretical framework for predicting the MMM performance is not yet available, therefore it is not straightforward to identify a priori which polymer/filler combination results in improved performances.

In this work, molecular simulations have been performed to study a MMM made of Matrimid® and ZIF-8 metal organic framework (MOF). The transport of different gas molecules like CO2 and CH4 has been analysed in the isolated phases as well as in a composite system made of two polymer layers with a ZIF-8 slab in between them. All simulations were performed with LAMMPS software and two methods were implemented to mimic the way experimental solubility and permeability tests are performed. The first method consists of putting the system in contact with two gas reservoirs at the same concentration at both sides of the membrane, then Molecular Dynamic (MD) runs are performed, which resemble the conditions of a pressure decay sorption experiment. The second method involves applying different concentrations for the two gas reservoirs and then Concentration Gradient Driven MD simulations [1] are performed, which resemble the conditions of a constant pressure permeation test.

Comparison with experimental dry polymer density and pure gas sorption isotherms guided the force field selection and validation of the simulation protocol. The single-phase systems and the composite ones were systematically compared in terms of transport properties, density profiles, local dynamics, and radial distribution functions. This allowed to highlight preferential interaction sites for the gas as well as interface effects on the polymer packing and chain dynamics, and how these affect the gas transport.

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Exploring the phase behaviour of confined water at high pressures using machine-learned interatomic potentials

Presenter: Ioachim Dusa
Affiliation: University of Cambridge, Cavendish Laboratory, TCM group

Water is predicted to turn metallic only under extreme compression, near 5 TPa. At such pressures water is expected to decompose before its band gap closes. This picture comes almost entirely from studies of bulk water. Inside planets, however, water is not entirely in bulk form. It is squeezed into thin layers between minerals, in places such as the Earth's mantle and the interiors of ice giants.

Confining water into nanoscale layers changes this picture. Using machine-learning-accelerated simulations, we map the behaviour of water squeezed into a slit a few atoms wide, from ambient pressure to several hundred gigapascals. We find a series of ice structures with no bulk counterpart, and we show that confined water metallises roughly an order of magnitude below the bulk pressure, without decomposing. In the same regime it also becomes superionic, with liquid-like protons moving through a fixed crystalline oxygen framework.

The mechanism is geometric rather than chemical. Confinement forces the hydrogen atoms out of the plane, which delocalises the conduction states. Additionally, it leaves the oxygen atoms undercoordinated, holding lone-pair electrons which in bulk water would be pulled into symmetric bonds. Preserved by the confining geometry, these lone pairs rise in energy under compression, and the two effects together close the gap at far lower pressure than in bulk.

These pressures are now within experimental reach. The confined transition near 500 GPa sits within range of modern diamond anvil cells, unlike the terapascal regime that bulk metallisation would require. More broadly, combining two-dimensional confinement with high pressure opens a route to new structural and electronic phases with no bulk equivalent.

Calcium carbonate Nanoparticle Stability

Presenter: Colin Freeman
Affiliation: University of Sheffield

The nucleation, crystallisation and growth of calcium carbonate remains a debated subject. The divalent charges of the cations leads to very slow dynamics which makes simulation of any processes difficult without applying biasing tools. These tools can be extremely powerful but can also suffer from exploring non-physical systems that do not give us the necessary insight into the real chemical behaviour. The whole process is made more complicated by the stability of a hydrated amorphous phase of calcium carbonate that further causes a lag in the formation of the crystalline phases. We have present a range of molecular dynamics simulations examining a range of different nanoparticles of calcium carbonate in solution. We examine these particles, of varying size, composition and shape to understand the stability and relaxations of these systems. By using a range of different tools to study structural behaviour we are able to determine a potential critical size range for the stability of calcium carbonate nanoparticles indicating the potential size of the nucleus.

Molecular dynamics investigation of polyhydroxyalkanoates for food packaging

Presenter: Janani Gangodawila
Affiliation: University of Strathclyde

Polyhydroxyalkanoates (PHAs) are renewable, biodegradable polymers with significant potential as sustainable alternatives to petroleum-based plastics. Among them polyhydroxybutyrate (PHB) has attracted particular interest due to its biocompatibility, non-toxicity, crystallinity and favourable barrier properties. However, its wider application is limited by brittleness, poor thermal stability during processing and restricted mechanical flexibility. Copolymerisation, incorporation of fillers and plasticisers offer routes to tailor crystallinity, microstructure and material performance. Though experimental studies have extensively examined the thermal, mechanical and structural properties of modified PHA systems, molecular level understanding of how composition and additives influence gas transport and barrier behaviour remains limited. In this study all atom molecular dynamics simulations are using to investigate the structural and dynamic properties of PHA-based polymers, with the long term aim of understanding gas diffusion in crystalline, amorphous and modified PHB, PHV and PHBV systems. Initial simulations were performed on amorphous PHB systems containing polymer chains of 10 monomers of 3-hydroxybutaric acid units. Using the General Amber Force Field (GAFF2), the simulated PHB density at 300 K was 1.13 $\pm$ 0.01 g cm-3, which was in good agreement with experimental and published simulation values. The calculated radius of gyration and end-to-end distances were also consistent with scaled literature values for comparable PHB chain lengths. The glass transition temperature was approximately 351 $\pm$ 17 K in this model, consistent with literature values. Future work will investigate the effects of crystallinity, copolymer composition, filler and plasticizer distribution and water and oxygen diffusion. By integrating molecular simulations this study will help to understand structure-property relationships for designing compostable PHA-based films with improved mechanical and gas barrier performance for food packaging applications.

Polymer membranes molecular dynamics simulation for sub-nanometre iso-ionic nanofiltration

Presenter: Shaoyang Gao
Affiliation: 07536203838

Size exclusion alone is often insufficient to separate structurally similar molecular ions, particularly when their molecular weights and sizes differ only slightly. Janus membranes composed of oppositely charged layers provide an alternative separation mechanism by coupling steric confinement with intramembrane electrostatic fields. In this work, molecular dynamics simulations were used to investigate the mechanism of transport selectivity of a charged Janus membrane toward acetylsalicylic acid (ASA) and salicylic acid (SA), which differ in rejection by 73.2% despite a molecular-weight difference of only 42 Da.

Atomistic membrane models were constructed from oppositely charged TpPa-SO3H and TpEB COP layers to form a bilayer Janus membrane, umbrella sampling simulations were performed along the membrane-normal direction to obtain potential of mean force profiles for ASA and SA permeation. The resulting free-energy profiles reveal distinct thermodynamic barriers for the two molecules, indicating that membrane selectivity cannot be explained by molecular size alone. The simulations show that intramolecular charge shielding plays a central role in controlling transport. ASA and SA exhibit different hydrogen-bonding patterns and solvent-shell reorganisation along the permeation pathway, which modifies the degree of charge exposure experienced by the Janus membrane. Charge-shielded species experience a lower free-energy penalty during membrane crossing, whereas more exposed charge leads to stronger electrostatic and solvation penalties. These molecular-level results support a size-gated charge-shielding mechanism, in which structurally similar iso-ions are separated by differences in effective charge density rather than size alone.

Polymers for Energy Transition: A Molecular Simulation Study of H_2 Transport in Semi-Crystalline Polymer Liners

Presenter: Hasan Ismaeel
Affiliation: University of Edinburgh

Authors : Hasan Ismaeel1,2 , Eleonora Ricci1,2, Omar Atiq2,3 , Perla Gavagni2,3 , Marco Baschetti2,3 , Maria Grazia DeAngelis1,2,3*

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Abstract:

Safe storage of compressed hydrogen is essential for accelerating the hydrogen energy transition. Type IV storage cylinders [1], which consist of polymer liners wrapped with carbon fibre-reinforced composites, offer a cost-effective solution for hydrogen storage. The selection of polymer liners with low hydrogen permeability is therefore critical for ensuring both storage efficiency and safety. In addition, a key failure mechanism in these tanks can occur during service cycles, where rapid depressurization may induce blistering in the polymer liner. This phenomenon is associated with the rapid expansion of sorbed gas within the liner and is often manifested through cracking and whitening of the material [1]. Therefore, elucidating high-pressure H_2 permeation in polymer liners is vital for guiding material selection and enabling safer, more reliable hydrogen storage technologies.

In this work, we leverage molecular simulations to predict and provide mechanistic insights into the diffusivity and solubility of H_2 in semi-crystalline polyphenylene sulfide (PPS). Specifically, we investigate H_2 transport using a hybrid simulation approach, in which Grand Canonical Monte Carlo (GCMC) simulations are employed to predict gas loading, while Molecular Dynamics (MD) simulations are used to account for sorption-induced plasticization and swelling of the polymer matrix. The equilibrated gas-loaded system is then subjected to further NPT MD simulations, during which the mean-squared displacement of the gas molecules is tracked to compute their diffusivity within the polymer.

Through this work, we aim to provide molecular-level insights that complement our experimental campaigns, while also evaluating the potential of PPS as a barrier material in comparison with more widely used polymers, such as high-density polyethylene and polyamides.

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Ab initio free energy calculations for planetary interiors

Presenter: David Lewis
Affiliation: The University of Edinburgh

We cannot directly observe the inside of a planet. However, the observations we can make (atmospheric composition, gravitational field, magnetic field, etc.) are directly linked to the properties of the planetary interior. The thermodynamic equilibrium composition of a planetary interior can be calculated from the Gibbs free energies of its constituent materials. We can compute a material's Gibbs free energy at the extreme conditions of planet interiors using coupling-constant integration (CCI) and density functional theory (DFT). Thermally excited phases, such as superionic ice, are not well represented by standard reference systems such as the quantum harmonic oscillator, and therefore require bespoke reference systems. In this work, we test the suitability of the simple Einstein crystal, combined with non-interacting components, as an alternative reference system for these exotic high pressure, high temperature, states of matter.

Towards understanding the Soret Effect in Polymeric Liquids

Presenter: Kseniya Papchenko
Affiliation: University of Pau and the Adour Region

Mass diffusion in complex mixtures can be induced through the application of a suitable temperature gradient. This effect is known under the name of Ludwig-Soret effect, or thermodiffusion, or thermophoresis when referred to biological fluids. The extent and direction of the resulting concentration gradient depends on multiple effects, such as mixture composition and molecular weight difference of components and can be quantified by the Soret coefficient, also defined as the ratio between the thermodiffusion coefficient and the mass diffusion one [1,2].

To date, a lot of work has been done to investigate the Soret effect in binary gaseous and liquid mixtures both experimentally and computationally. On the other hand, the investigation of this effect in ternary mixtures and polymeric liquids is still quite limited, but of great practical interest for applications ranging from fluid storage and transport to food processing and biomedical industries [1].

While some effects, like Soret coefficient variation with the molecular weight of the polymer, have been investigated for several polymer–solvent systems, other phenomena, like the effect of tacticity or of copolymer structure (of great importance for polymer fractionation), are still lacking accurate description. This is due to limited availability of experimental data and intrinsic difficulty associated with investigation of ternary systems or polymeric systems at high polymer concentration.

Here, we use molecular analysis to investigate the Soret effect in polystyrene:toluene:cyclohexane (PS:Tol:cHex) mixture. Such mixture represents a suitable model system given the availability of experimental data for atactic PS. Another point of scientific interest is given by opposite sign of the Soret coefficient for PS:Tol, PS:cHex, and Tol:cHex mixtures, hence the coefficient of the ternary system is expected to be dependent on the Tol:cHex concentration of the binary solvent. Moreover, PS is an ideal candidate to investigate the influence of tacticity on thermodiffusion, providing the link between transport and interaction energy of components in the mixture. Here, we apply the Equilibrium and boundary-driven Non-Equilibrium Molecular Dynamics to investigate mixtures of isotactic, syndiotactic, and atactic PS at infinite dilution in Tol, cHex, and Tol:cHex at equilibrium and under the effect of the temperature gradient.

Keywords: thermodiffusion; Soret coefficient; polymeric liquids

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Investigating Interfacial Thermal Resistance and Effective Thermal Conductivity in Epoxidized Natural Rubber Composites

Presenter: Muhamamd Uzair Riaz
Affiliation: Technical University of Dresden

Effective thermal management in polymeric materials still represents a considerable challenge for emerging applications, such as wearable electronics, soft robotics, and sustainable composite systems, wherein flexibility and environmental compatibility are of utmost importance. This research utilizes non-equilibrium molecular dynamics (NEMD) simulations to examine interfacial thermal resistance (ITR) and effective thermal conductivity (keff) in bio-based PBS-ENR-PBS trilayer systems. Two varieties of epoxidized natural rubber, ENR-25 and ENR-50, with varying epoxide concentrations, are analyzed to clarify the influence of interfacial polarity and chemical reactivity. Interfacial heat transmission is systematically adjusted by including covalent transesterification crosslinks at the PBS-ENR interface, with concentrations ranging from 0 to 50%. Steady-state temperature profiles, heat fluxes, and density-based interface detection are employed to quantify layer-specific conductivities, interfacial temperature discontinuities, and total thermal resistance. The findings indicate that moderate crosslinking significantly improves interfacial phonon coupling and diminishes ITR in ENR-25 systems, but excessive crosslinking results in saturation due to constrained chain mobility. Conversely, ENR-50 demonstrates a faster onset of transport saturation due to its elevated inherent polarity and stiffness. The findings indicate that effective thermal transfer in soft, bio-based polymer interfaces results from a balance of molecular connection and segmental flexibility, offering design principles for thermally efficient elastomeric composites.

Exploring OpenFF and MACE Workflows for Developing Interatomic Potentials for PDMS

Presenter: Oliver Shepherd
Affiliation: Newcastle University

Modern approaches to force field design have the potential to transform the accuracy of polymer simulations. However, approaches such as those developed by the Open Force Field (OpenFF) Initiative tend to focus on organic chemistry and drug design applications, while machine learning interatomic potentials, such as MACE, have not been widely tested in the condensed phase. This project aims to evaluate multiple Molecular Dynamics (MD) workflows, including OpenFF and MACE based approaches, for amorphous polymer simulations. The project focuses on a representative Si-based polymer PDMS a widely used elastomeric material whose mechanical properties are highly sensitive to both the underlying potential and parametrisation strategies. The workflows will be analysed by their reproducibility, efficiency and ability to converge mechanical properties.

Integral Equations and Density Functional Theory for the cluster fluid phase of fluids with competing interactions

Presenter: Martin Sweatman
Affiliation: University of Edinburgh

Fluids with short-ranged attractive (SA) interactions and long-ranged repulsive (LR) interactions, often called SALR fluids, are known to form clusters of particles at low concentrations for suitable combinations of SALR parameters. These clusters can appear to behave like a stable dispersion of liquid-like droplets. SALR fluids are, therefore, often considered a reasonable model for some biological molecules, such as proteins, and other large molecules that are also known to form large stable clusters in solution. Their clustering behaviour could also be useful in describing the formation of membraneless organelles within biological cells, for which the current preferred model in the research literature is liquid-liquid phase separation (LLPS) - even though LLPS does not naturally form liquid-like droplets at equilibrium.

Due to their strong concentration fluctuations over multiple length scales, SALR cluster fluids have proved quite challenging to model theoretically using standard methods, such as integral equations and density functional theory. Here, some recent progress in this area towards obtaining an accurate density functional theory (DFT) for the cluster fluid phase is presented [1]. A key input into this weighted DFT is accurate knowledge of the pair direct correlation function along an isotherm. This can be generated using integral equation methods. Because standard integral equation closures and/or Picard iteration solution methods for these clustered states often fail, ChatGPT5 was used to help design a more robust method that can overcome such ”stiffness” problems for some closures [2].

[1]M.B. Sweatman, submitted to Molecular Physics, 2026.

[2]M.B. Sweatman and J. Tan, submitted to Molecular Physics, 2026.

D_ATA: A Universal Atom Typer and Analyser for Characterising Non-Bonded Atomic Interactions

Presenter: Chin Yong
Affiliation: STFC Daresbury Laboratory

Understanding non-bonded interactions in atomistic systems — hydrogen bonds, hydrophobic contacts, van der Waals dispersive forces, and aromatic π-system interactions — is central to rationalising the characteristics behaviour of molecular systems including protein folding, molecular bindings and recognition, and structural stability. However, extracting meaningful, chemically interpretable, and computationally searchable interaction information from molecular data remains a significant challenge.

Here we present D_ATA [1], Atom Typer and Analyser, a program for the identification, annotation, and quantification of non-bonded atomic interactions in any atomistic system, independent of the simulation package or force field scheme used to generate the trajectory. D_ATA integrates two unique complementary capabilities developed at Daresbury Laboratory. The first is DL_F Notation [2], a universal atom typing scheme that assigns every atom in a molecular system a self-explanatory, chemistry-containing label. With coverage of more than 440 Chemical Groups, DL_F Notation covers a wide range of chemical space and provides unambiguous chemical identity for every atom in the system. The second is DANAI (DL_ANALYSER Notation for Atomic Interactions) [3], a structured, text-based language construct for annotating non-bonded interactions between Chemical Groups. DANAI expressions are human-readable, chemically interpretable, and amenable to computational query, transforming interaction data from complex numerical outputs into a structured, searchable dataset.

The interaction classification layer is user-configurable through the DLF_map library file, allowing users to add new Chemical Group combinations, redefine interaction types, or extend coverage to newly relevant molecular classes — without modifying or recompiling the software. Crucially, the underlying atom typing layer remains universal and fixed, guaranteeing that all results are chemically reproducible and directly comparable across force field schemes and simulation packages.

References

[1] D_ATA — Atom Typer and Analyser, version 2.0. https://www.ccp5.ac.uk/D_ATA (2026).

[2] Yong, C. W. J. Chem. Inf. Model. 2016, 56, 1405–1409.

[3] Yong, C. W.; Todorov, I. T. Molecules 2018, 23, 36.

ML-PEG: ML Performance and Extrapolation Guide

Presenter: Elliott Kasoar
Affiliation: STFC/University of Cambridge

Recent advances in machine learnt interatomic potentials (MLIPs) are revolutionising atomistic simulations, enabling results with accuracy comparable to ab initio calculations at significantly greater time and length scales. In addition to improved model architectures, access to large, high-quality datasets has enabled the creation of foundational models, trained on sufficiently diverse data to act as a general-purpose model, or starting point, for applications ranging from molecules to proteins. However, as model architectures continue to develop, and new training data becomes available, it has become clear that we are limited in our current methods for rigorously benchmarking foundational MLIPs. Many frequently cited benchmarks are becoming saturated in their scores, focus on a narrow range of systems, such as bulk inorganic crystals, and favour low energy and force errors, rather than more complex physical properties. These limitations inhibit meaningful comparisons of state-of-the-art models, as well as our ability to explain quite diverse performances of models when studying different properties or systems. To address this, we introduce the Machine Learning Performance and Extrapolation Guide (ML-PEG), a hierarchical, customisable, interactive interface, through which the results of benchmarks spanning a wide range of material/molecular applications and physical properties can be examined, ranging from a single numerical score to visualisation of individual atomic structures from a dataset.

uMOF: A Universal Database, Benchmark, and Machine Learning Interatomic Potentials for Metal-Organic Frameworks

Presenter: Alin Marin Elena
Affiliation: Scientific Computing Department, Science and Technology Facilities Council, Daresbury Laboratory, UKRI

Foundation machine learning interatomic potentials (MLIPs) deliver near-ab-initio accuracy at a fraction of the computational cost, yet their promise for Metal-organic Frameworks (MOFs) remains largely unrealized as large unit cells make first-principles training data expensive to generate, fine-tuned models are scarce, and experimentally grounded benchmarks are scarcer still. We introduce uMOF, a three-part contribution addressing this gap. First, we release the largest and most accurate density functional theory (DFT) dataset for MOFs to date, computed at the r^{2}SCAN-D4 level of theory across 85,524 configurations spanning 19,950 unique frameworks and 79 elements, covering empty and gas-loaded structures, geometry optimizations, equations of state, and finite-temperature molecular dynamics (MD). Second, we release a literature-mined benchmark of 3,986 verified property values (3,146 experimental) extracted from 626 papers by a seven-stage, checkpointed multi-pass large language model (LLM) pipeline, linked to more than 650 crystallographic information files (CIFs). Third, we release two universal MLIPs for MOFs, uMOF-MH and uMOF-POLAR, fine-tuned from two architecturally distinct MACE foundation models on the uMOF dataset. On near-equilibrium, "Tier-1" properties (bulk modulus, phonon-derived heat capacity) the uMOF models perform comparably to existing foundation and fine-tuned baselines. On harder, dynamics-sensitive properties like gas adsorption enthalpies via Widom insertion and adsorption isotherms, the uMOF models outperform every baseline we test, including MOF-specialized gas-capture models trained on datasets up to three orders of magnitude larger, cutting error by more than 80% to within experimental uncertainty. We trace this advantage to the physical diversity of the training data and to level of theory where a small (1.7%) fraction of MD simulations is decisive for MLIP stability, and r^{2}SCAN-D4 captures guest-MOF and metal-linker interactions that GGA-level (PBE) datasets miss. We release the dataset, benchmark, and models as a reproducible standard for MLIP development in reticular chemistry.

Data-Driven Surface Engineering and Bonding Evolution of Diamond-Like Carbon Coatings for Biomedical Applications

Presenter: Anam Ijaz
Affiliation: Heriot-Watt University

Diamond-like carbon (DLC) coatings are widely used to improve performance and biocompatibility of engineering and biomedical devices. In general, DLC exhibits a nanoscale roughness with nano topography, however, they are sensitive to manufacturing parameters. For example, role of bias voltage and gas pressure significantly influences coating growth when made with standard Physical Vapor Deposition (PVD) or Plasma Enhanced Chemical Vapor Deposition (PECVD) methods. A detailed incremental study requires significant resources and time to identify manufacturing parameters for suitable roughness and topography. This research presents a data-driven framework that predicts the nano-topography of DLC coated substrates, structural evolution and surface characteristics under different deposition conditions. Emphasis is placed on nano-scale roughness as a key factor influencing anti-microbial behaviour and other application-specific surface functionalities. Molecular dynamic simulations are used for observing the interconnected structural and topographical descriptors that are important for controlling and monitoring the biocompatibility and bacterial adhesion on biomedical surfaces.

Materials Modelling at AWE

Presenter: Ben Ellis
Affiliation: 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 and to explosives. A widely applicable question within these materials, concerns how they age over many years and specifically how this affects their material properties. To develop the detailed mechanistic understanding required for a robust and consistent predictive capability, model representations are built using a range of different computational techniques and tested against experiment where possible. Often several computational techniques, from electronic structure theory to finite element modelling, are required to develop the necessary model representations. To support such projects AWE utilises both internal and external research activities. External collaborations allow AWE to benefit from the wide range of modelling expertise available more broadly in the academic community and allow for the trial and development of advanced technical methods before they are employed internally.

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