Thomas Young Centre Student Day 2025

Wednesday 11th June 2025

09.30 to 18.00

Arts Two LT and foyer space, Queen Mary University of London

Time	
09.30 – 10.00	Welcome with Tea & Coffee
10.00 – 10.05	Opening remarks
	Student Talks
10.05 – 10.25	Impact of pathogenic missense mutations on the dynamics of human skeletal myosin ***Ka Fu Man, Queen Mary University of London***
10.25 – 10.45	First Principle Approach to Calculate High-pressure Phase Diagram of Binary Alloy in Low-solute Concentration Limit ***Shambhu Bhandari Sharma, University College London***
10.45 – 11.05	OptaDOS Photoemission - Dissecting Photocathode Materials and their Surface Chemistries ***Felix Mildner, Imperial College London***
11.05 – 11.25	Towards accessible wavepacket dynamics of photo-induced processes ***Léon Cigrang, University College London***
11.25 – 11.55	**Tea & Coffee & posters**
11.55 – 12.15	Tunable Polarisation in $PbTiO_3$: The Role of Hydrogen Coverage and Film Thickness ***Nisrine Sakaki, London South Bank University***
12.15 – 12.35	Towards Conservation of the Quantum Boltzmann Distribution in Mapping Methods: A Normal Mode Approach ***Lauren Cook, University College London***
12.35 – 12.55	Modelling point defects at device operating conditions ***Irea Mosquera Lois, Imperial College London***
12.55 – 14.00	**Lunch & Poster Session**
14.00 – 14.20	Computational Modelling of Charge Trapping and Defect Properties in Amorphous and Crystalline Gallium Oxide ***Chaiyawat Kaewmeechai, University College London***
14.20 – 14.40	Data-Driven Design of Photovoltaics, Thermoelectrics and Transparent Conductors ***Ruiqi Wu, Imperial College London***
14.40 – 15.00	A study of CO2 adsorption in Cucurbit[n]urils ***Gowan Whalley, University College London***
15:00 – 15:30	**Tea & Coffee & posters**
	Plenary Speakers
15.30 – 16.00	An Industrial Perspective on the Challenges and Opportunities in Multiscale Materials Modelling **Davide Di Stefano, Ansys, Inc.**
16.00 – 16.30	Making Disordered Proteins Druggable **Thomas Löhr, Bind Research**
16.30 – 18.00	**Closing Remarks, Final Poster Session, Prize Announcement & Reception**

Final year student presentations

Abstracts

Impact of pathogenic missense mutations on the dynamics of human skeletal myosin

Ka Fu Man, Queen Mary University of London

Congenital myopathies are typically an early-onset genetic diseases characterised by muscle weakness.1 The overall prevalence is estimated to be 1.62:100,000 in a recent meta-analysis.2 Myosinopathies represent a class of congenital myopathies associated with mutations in various myosin isoforms.3 One of the most abundant myosin isoforms in skeletal muscle is known as the fast type IIa myosin (MYH2). Pathogenic missense mutations can alter the intrinsic dynamics of a protein. To date, ten missense mutations have been identified in the MYH2 gene, all located within the motor-neck domain. However, no therapeutic treatment currently exists.

Omecamtiv Mecarbil (OM) has gathered significant research interest since its introduction as first-in-class allosteric cardiac muscle activator. A recent molecular dynamics (MD) study from our group has rationalised the selectivity of OM in cardiac myosin over skeletal myosin.4 A hydrophobic subpocket adjacent to the OM binding pocket was identified specifically in the skeletal isoform, which could be leveraged to design small molecules selective to skeletal myosin.

An open question remains whether pathogenic missense mutations affect the dynamics of MYH2 and how these changes might propagate to the OM binding site. In this work, we found significant differences in three pathogenic missense mutants compared to the wild-type MYH2 isoform: i) the relay helix, a key element of myosin function and partially involved in OM binding, shows larger motions and ii) the dynamic correlations between the domains surrounding OM are weaker. Consistent with these findings, the OM binding pocket volume has larger fluctuations and a hydrophilic subpocket is more accessible during the mutant simulations compared to the wild type. These results can be used in the future to guide in silico drug design for the targeting of skeletal myosin mutants.

1. Jungbluth et al., Nat Rev Neurol 2018, 14 (3), 151-167
2. Huang et al., Front. Neurol. 2021, 12, 761636
3. Tajsharghi et al., Neuropathol 2013, 125(1), 3-18
4. Antonovic et al., Biophysical Journal 2023, 122(1), 54-62

First Principle Approach to Calculate High-pressure Phase Diagram of Binary Alloy in Low-solute Concentration Limit

Shambhu Bhandari Sharma, University College London

Phase diagrams are crucial to the design of new materials, to understand their phase stability and metastability under different thermodynamic conditions, such as composition, temperature, and pressure. Here, we use an ab initio approach to study the phase diagram of a binary alloy within the low concentration limit of a solute. Using the ab initio molecular dynamics calculations based on density functional theory, we estimate the solute partitioning ratios in solid–liquid phase equilibria. The chemical potential difference between the solvent and solute atoms in both solid and liquid phases is calculated using thermodynamic integration. As an illustration of the techniques, we have applied this method to reproduce the phase diagram of the Al–Mg alloy at zero pressure. We also compute the ab initio solid–liquid coexistence curve of pure Al by applying the phase-coexistence method with the free energy correction technique. The calculated results are in close agreement with the experiment, demonstrating the reliability of the models.

OptaDOS Photoemission - Dissecting Photocathode Materials and their Surface Chemistries

Felix Mildner, Imperial College London

Photocathodes are vital for the operation of free electron lasers (FELs) and other ultra-short, pulsed electron sources. The main challenges in the design of efficient photocathodes are balancing the quantum efficiency (QE) and intrinsic emissivity of the material and cathode device itself.

With the advance of electronic structure theory and code packages the atomistic modelling of photocathodes has also found success in contributing to the design of efficient photocathodes. One can estimate the photoemission of a material, by studying the bulk electronic structure. The detailed chemistry of the surface and its influence on the emission, however, is a factor that has not been widely considered in modelling efforts up to now.

We have developed a photoemission focused module extending the functionality of the widely used and freely available OptaDOS code package. This module can compute a surfaces photoemission taking into account the detailed chemical environment of each site within the surface.

OptaDOS is designed to take ab initio electronic structure data and compute a material's relevant optical and electronic properties. Using the added functionality, the contribution of layers to the total QE in a simulated surface and the total emissivity can be calculated. This allows the deconvolution of contributions from different sites in defective surfaces or systems with heterostructures, such as adsorbed gasses or deposited materials.

Towards accessible wavepacket dynamics of photo-induced processes

Léon Cigrang, University College London

Non-adiabatic quantum dynamics simulations are powerful tools used to describe the ultrafast nuclear motion of molecules by solving the time dependent Schrödinger equation. Specifically, these calculations are often used to study photochemical processes such as dissociation or isomerisation reactions and can provide great insights for the interpretation of experiments studying the same phenomena. The accuracy provided by such methods comes at a great cost however, in terms of computational effort, but also a lack of accessibility. Addressing this first bottleneck is done, as usual, by introducing various approximations to reduce the cost of the calculations and allow simulation of larger systems. Specifically, this talk presents work towards the description of solvated systems using wavepacket dynamics. The issue of accessibility on the other hand, is not often addressed. Some important considerations will be made surrounding the practical challenges associated with the field of quantum dynamics. Additionally, recent community-wide efforts that aim to solve big outstanding challenges of the field are highlighted. Overall, this presentation will provide examples of the impressive capabilities of the current state of the art of quantum dynamical modelling, while also emphasising the challenges that lie ahead on the road towards maturity.

Tunable Polarisation in $PbTiO_3$: The Role of Hydrogen Coverage and Film Thickness

Nisrine Sakaki, London South Bank University

Ferroelectric materials are a class of functional materials characterised by spontaneous electric polarisation that can be reversed by an external electric field. This property makes them highly attractive for a variety of applications, including non-volatile memory devices, sensors, actuators, and capacitors. Among them, lead titanate ($PbTiO_3$, PTO) and barium titanate ($BaTiO_3$, BTO) are widely studied due to their high polarisation and tunable properties.

In this study, we focus on PTO-based systems to investigate the influence of surface hydrogen deposition on ferroelectric polarisation. We examine PTO structures of varying thicknesses to understand how hydrogen adsorption affects both the magnitude and direction of polarisation. Additionally, we analyse larger supercells with different hydrogen coverage percentages to assess the impact on polarisation behaviour.

Our results reveal that increasing hydrogen coverage leads to a notable enhancement in polarisation in larger PTO systems. Furthermore, hydrogen deposition can induce a polarisation direction switch for systems with varying thicknesses, with thicker PTO films (e.g., increasing from 3 to 7-unit cells) showing a significant rise in polarisation magnitude. These findings highlight the critical roles of both surface chemistry and structural thickness in modulating ferroelectric behaviour, offering valuable insights for the design of advanced ferroelectric devices.

Towards Conservation of the Quantum Boltzmann Distribution in Mapping Methods: A Normal Mode Approach

Lauren Cook, University College London

Simulation of nonadiabatic dynamics is complex due to the coupling between the nuclear and electronic degrees of freedom. Often mapping methods are utilized, where the quantum subsystem is mapped onto classical variables that are propagated with classical mechanics. One can write out a list of desirable criteria for a mapping method, including conservation of the quantum Boltzmann distribution (QBD), reproduction of Rabi oscillations, classical scaling with system size and a derivation from exact quantum dynamics. However, none of the existing methods satisfy all of these.

In single surface dynamics, such a method exists that satisfies all the criteria, known as Matsubara dynamics. The QBD conservation arises due to the use of nuclear normal modes and is proven algebraically. However, the nonadiabatic counterpart (J. Chem. Phys., 2021, 154, 124124) that also uses nuclear normal modes does not conserve the QBD. We suggest that additionally using electronic normal modes for the electronic subsystem may lead to conservation of the QBD for nonadiabatic dynamics.

Here, we will discuss the use of electronic normal modes for an electronic-only system and identify how better understanding electronic normal modes has significantly improved the outlook for developing a method that satisfies all the desirable criteria.

Modelling point defects at device operating conditions

Irea Mosquera Lois, Imperial College London

Point defects are ubiquitous in solid-state compounds and play a key role in properties like ionic conductivity, solar cell performance and catalytic activity. The standard approach to modelling defects is to calculate their properties at 0 K, ignoring atomic vibrations and defect structural changes [1-4] that occur at device operating temperatures [5]. While this reduces the computational cost, it can miss important thermal effects and result in incorrect predictions.

To address these limitations, we use machine learning force fields to model defects at operating conditions, thus describing their dynamics and equilibrium properties over longer length and time scales than previously possible. Our work on point defects in CdTe and $CsPbCl_3$ has shown that thermal effects can significantly change the predicted defect properties, from equilibrium concentrations [6] to electronic behaviour, compared to the conventional 0 K approximation. These shifts can lead to incorrect predictions of which defects form under different synthesis conditions and how detrimental they are to device performance, thus making the consideration of thermal effects key for more accurate defect models.

[1] I. Mosquera-Lois and S.R. Kavanagh, Matter, 2021
[2] I. Mosquera-Lois, S.R. Kavanagh, A. Walsh and D.O. Scanlon, J. Open Source Softw., 2022
[3] I. Mosquera-Lois, S.R. Kavanagh, A. Walsh and D.O. Scanlon, npj Comp Mater, 2023
[4] I. Mosquera-Lois, S.R. Kavanagh, A.M. Ganose and A. Walsh, npj Comp Mater, 2024
[5] I. Mosquera-Lois, S.R. Kavanagh, K. Tolborg, J. Klarbring and A. Walsh, Chem Soc Rev, 2023
[6] I. Mosquera-Lois, J. Klarbring and A. Walsh, Chem. Sci., 2025

Computational Modelling of Charge Trapping and Defect Properties in Amorphous and Crystalline Gallium Oxide

Chaiyawat Kaewmeechai, University College London

Crystalline gallium oxide is recognised as a potential candidate for high-power electronics and UV photodetector applications because of its ultra-wide bandgap of around 5 eV and high critical breakdown field. In addition, amorphous gallium oxide has been considered for use in memristor applications.

Charge trapping and defects can significantly influence the reliability and performance of these devices. Therefore, we investigate the intrinsic defects of gallium oxides, i.e., charge trapping, oxygen vacancy (VO), and interstitial defects (Oi), using the density functional density. The results reveal that holes can be trapped in both the amorphous and crystalline phases, forming a self-trapped hole on the oxygen atoms, whereas electron trapping does not occur in this material. Additionally, introducing a second hole into the system allows for the formation of a hole bipolaron (O-O dimer). For VO defects, the deep charge transition level between the +2 and 0 charge states varies significantly depending on the crystal phase and the coordination environment of the surrounding atoms. In the case of Oi defects, results indicate that Oi atoms can form O-O dimers in split configurations in the neutral and +1 charge states. At high Fermi levels, these dimers are capable of trapping additional electrons, subsequently breaking a bond to yield an O ion in the -1 and -2 charge states. Furthermore, the O--O dimer exhibits the ability to migrate to adjacent atomic rings through bond-breaking and rotational mechanisms.

By combining knowledge of intrinsic defects, the mechanism behind defect creation can be formulated. The Frenkel pairs (FPs), consisting of VO and Oi are considered a consequence of hole bipolaron formation. The activation energies for the creation of FPs via the formation of hole bipolarons are significantly lower than those observed in the pristine structure.

Data-Driven Design of Photovoltaics, Thermoelectrics and Transparent Conductors

Ruiqi Wu, Imperial College London

The discovery of new materials has driven advances in energy conversion and storage, including batteries, photovoltaics, thermoelectrics and transparent conductors. Recently, Google released the GNome[1] dataset of hypothetical compounds, built on an unbiased screening of chemical space, which identified thousands of novel potentially stable inorganic materials. However, the true stability of these compounds remains unclear, and their functional properties have yet to be evaluated for energy applications. In this work, we carry out a large-scale high-throughput screening of the GNome dataset. We employ hybrid density functional theory to robustly evaluate the optoelectronic properties of over 600 compounds, selected according to their earth-abundant and non-toxic compositions and predicted bandgaps. Based on this, we ranked the compounds based on their suitability for photovoltaics, thermoelectrics and transparent conductor applications. To provide reliable predictions of materials stability, we comprehensively ensure the predicted materials are the true thermodynamic ground state through ab initio random structure searching, while, dynamical stability is assessed through vibrational properties. For the most promising candidates, we obtain the intrinsic defects and electronic transport properties to guide experimental device design. Our work identifies several novel earth-abundant candidates with state-of-the-art performance in energy applications.

[1] Merchant, A., Batzner, S., Schoenholz, S.S. et al. Scaling deep learning for materials discovery. Nature 624, 80–85 (2023). https://doi.org/10.1038/s41586-023-06735-9

A study of CO2 adsorption in Cucurbit[n]urils

Gowan Whalley, University College London

Cucurbit[n]urils have been shown experimentally to be very proficient absorbers of CO2.1 Work has been carried out to model the uptake of CO2 within cucurbit[n]uril hosts in vacuo and in crystalline phases with simulations being carried out to examine CO2 adsorption amounts, binding sites and binding dynamics. These have been carried out using Molecular Dynamics (MD) and Monte-Carlo approaches.

Monte-Carlo and Molecular dynamics simulations have been applied to a series of sizes of the curcurbit[n]uril family macro-cycles as hosts, aiming to estimate the behaviour of both single macro-cycles and extended crystals in a CO2 environment. Crystal structures of macro-cycles have either been extracted from the Cambridge Crystallographic Database2 or generated using Simulated Annealing in a GAFF2 forcefield, chosen due to its superior performance as a general forcefield in host dynamics.3 First, the models have been challenged to replicate experimental observations of CO2 adsorption into experimentally available macro-cycle crystals, then extrapolated to and compared against those generated by simulated annealing. Simulations have shown a general increase in binding affinity as the macro-cycle increases in size.

Accompanying this work, the kinetics of CO2 absorption into the cavity has also been investigated and how the crystal packing effect the dynamics of binding and access to the cavity under different conditions. Providing insight into how CO2 absorption differs between the amorphous and crystalline phases of the material.

1 H. Kim, Y. Kim, M. Yoon, S. Lim, S. M. Park, G. Seo and K. Kim, J. Am. Chem. Soc., 2010, 132, 12200–12202.
2 C. R. Groom, I. J. Bruno, M. P. Lightfoot and S. C. Ward, Acta Crystallogr B Struct Sci Cryst Eng Mater, 2016, 72, 171–179.
3 X. Wang, Z. Huai and Z. Sun, Molecules, 2023, 28, 5940.

Plenary Speakers

Davide Di Stefano, Ansys, Inc - An Industrial Perspective on the Challenges and Opportunities in Multiscale Materials Modelling

Materials are at the core of engineering simulations, directly influencing the accuracy and reliability of performance predictions. However, materials data is often treated as static input derived from costly and time-consuming experimental testing. Increasing material complexity and performance demands require more precise, adaptable, and predictive data. Multiscale materials modelling offers a powerful solution to the problem, providing mechanistic insights that can contribute to the reduction of experimental efforts, and enhancing accuracy and efficiency. Despite its promise, multiscale modelling is not yet widely adopted in industry.

In this talk, we will provide an industrial perspective on the open challenges in fulfilling the "multiscale promise" and share examples of effort within Ansys to address these challenges. Examples will include physics-based workflows for multiscale modelling, use of machine learning for scale-bridging, and advanced multiscale characterization techniques for calibration and validation.

Thomas Löhr, Bind Research - Making Disordered Proteins Druggable

We are a UK-based not-for-profit Focused Research Organisation (FRO) committed to improving patient outcomes by turning disordered proteins into viable drug targets.

Many incurable diseases (e.g., cancer, neurodegeneration) involve biomolecules called 'disordered proteins'. Considered 'undruggable' by the mainstream pharmaceutical industry, disordered proteins continuously change their three-dimensional shapes and lack long-lived sites with which drug-molecules can interact.

Our mission is to make disordered proteins druggable. We are screening millions of disordered protein/drug-molecule pairs to learn the rules of drugging disordered proteins.

Building on our expertise and working with academic and industrial partners, we are leveraging cutting-edge biology, engineering, and AI to deliver new drugs and tools. We are building comprehensive datasets of disordered protein-drug interactions to create public assets to fuel AI models and accelerate the discovery process. To accomplish this in a manner for maximum societal benefit, we have established a Focused Research Organisation (FRO), a fully independent not-for-profit entity dedicated to this goal.

All Year Student Posters

Poster Number	Name	Poster Title
1	Marcus Allen	A novel 'moment'-based GW algorithm for molecules and solid
2	Iona Anderson	A data driven approach to enhancing specific capacity in n-type OMEICs for energy storage
3	Mateja Batelic Jankovic	Bright isolated XUV attopulse generation through high-order frequency mixing process
4	Sophia Ber	Investigation of Molecular Determinants of Gating in K2P Channels via Molecular Dynamics Simulations
5	Marcus Brady	Nonadiabtic Dynamics for Organic Molecules
6	Wenxuan Cai	Modelling the core electron binding energy at metal oxide surface
7	Pietra Cerqueira Diaz	Modelling Hair Lubrication in the Presence of Additives
8	Christopher Tat Shun Cheung	Coexisting charge density waves in twisted bilayer NbSe2
9	Sam Crowhurst	How did the ion cross the channel? A molecular dynamics investigation into DEG/NaC channel function
10	Wei Dai	ANNalog - Generation of MedChem-similar molecules
11	Merve Dene	Understanding the Hexagonal Boron Nitride / Re(0001) Interface: Experimental and Computational Analysis
12	Aaron Dines	Thermal Equilibrium in Coupled Trajectory Mixed Quantum-Classical Dynamics
13	Jordan Edwards	Modelling the Chemical Interface Damping of Surface Plasmon Polaritons
14	Stylianos Iliadis	Druggability-enhanced structural chemogenomics approaches to navigate the dopamine GPCR-ligand interaction space
15	Michael Ingham	Describing excited states of covalently connected crystals with cluster and embedded cluster approaches: Challenges and solutions
16	Filip Ivanovic	Non-adiabatic Dynamics Simulation of Charge Generation in Organic Solar Cells
17	Kit Joll	From Free-Energy Landscapes to Field-Driven MD: A Machine-Learning Approach
18	Ewen Jones	Finetuning MACE Machine-Learning Potentials for Studying the Binding Modes of a RuP dye photosensitiser on TiO2 nanoparticles
19	Aadi Konidena	Hubbard Interactions and the CISS Effect in Helical Molecules
20	Wuyang Lin	Screening Nitrogen-Coordinated Single Atom Catalysts on Armchair Carbon Nanotubes for Enhanced Electrochemical CO2 Reduction to C1 Products
21	Miguel Luque Canete	Phonon-Limited Conductivity of Topological Surface States in Bi2Se3 and of Bulk States in Graphene
22	Isaac Mackley	Affects of nitrogen incorporation in hafnia
23	Ivan Manosa	Structural Basis of Inward Rectification in the hERG Cardiac Potassium Channel

24	Md Maruf Mridha	Computational analysis of the ground state properties of g-C3N4
25	Andras Petho	Investigating the conductivity of Multi-Heme Cytochromes
26	Klara Pribanova	Benchmarking Machine Learning Potentials to Study Melanin Oligomers
27	Aritra Roy	ComProScanner: Multi-agent Based Composition-Property Data Extraction Framework
28	Ollie Russell	Investigation the method of conductance in highly conducting cable bacteria
29	Elisavet Tsakelidou	Computational Insights into Magnesite Reactivity for CO2 Sequestration Optimization
30	Ingvars Vitenburgs	Stochastic Coherent State Path Integral Approach to Electrons in a Solid
31	Zijie Wang	Theoretical characterization of the Wurzite and Zincblende GaN stacking faults
33	Yu-Yuan (Stuart) Yang	Holo-like conformation selection using a computer vision-based deep-learning model

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