TYC Postgraduate Student Day 2026

9:30 am – 6 pm, Wednesday 10 June

Great Hall, King’s College London, Strand

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Final Year Abstracts

Phonon-Limited Conductivity of Topological Surface States in Bi_2Se_3

Miguel Luque Canete, King's College London

Topological insulators, such as Bi2Se3, exhibit topological surface states (TSS) with promising applications where understanding their electronic transport properties is essential. At room temperature, electron-phonon interactions could significantly impact the conductivity of TSS, yet the dominant mechanisms of electron-phonon scattering remain unclear. In this work, we develop and validate a framework to compute the phonon-limited conductivity of the Bi2Se3 TSS using the Boltzmann transport equation in the relaxation time approximation. We include scattering with acoustic and non-polar optical phonons via deformation potential coupling. Acoustic phonons are obtained from the anisotropic elastic continuum equations, and non-polar optical phonons from an extended slab model and density functional theory. In addition, we introduce an anisotropic dielectric continuum model to account for long-wavelength optical phonon scattering. All physical parameters entering the framework can be obtained from ab-initio calculations. Applying the framework to Bi2Se3 TSS, we quantify scattering rates arising from distinct phonon modes and evaluate their contributions to the temperature-dependent transport properties of TSS.

Resonant Doping in Sb(V)-based Oxides for High-Mobility Transparent Conductors

Ke Li, University College London

Transparent conducting oxides (TCOs) combine high conductivity with optical transparency, underpinning a wide range of optoelectronic technologies. ZnSb2O6 and Sb2O5 were recently realized and predicted as an earth-abundant TCO with Ga and F doping. [1,2] Resonant dopants are attractive for TCO applications as their donor d-states sit well above the conduction band minimum, preserving high mobility while enabling high carrier concentrations.

In this work, we employ PBE0 functional density functional theory to investigate the resonant doping behaviour of Sc in ZnSb2O6 and of Mo and W in Sb2O5 and ZnSb2O6. [2,3] Both materials have wide n-type doping windows, which are optimal for extrinsic dopants incorporation. In ZnSb2O6, Sc acts as a resonant dopant, with the unfolded band structure showing its 3d states positioned ~ 4.5 eV above the conduction band edge. This preserves the dispersive Sb 5s at CBM and yields an overall electron concentration of 10^19 – 10^20 cm^-3, showing n-type degenerate transparent conducting oxide behaviour. Mo and W were chosen as potential candidates to substitute the Sb site for both materials, based on the success of Mo doping in In2O3 and W doping in SnO2.[4,5] Although the substitution defects residing in the bandgap for Mo- and W-doped ZnSb2O6, they incorporate favourably in Sb2O5, where both substitution defects exhibit low formation energies and have localised d-states appearing above the CBM. These findings broaden the design principles for optimisation of Sb(V)-based transparent conductors.

1. Jackson, A. J, et al., ACS Energy Lett., 2022, 7, 3807-3816.
2. Li, K. et al., Chem. Mater., 2024, 36, 2907-2916.
3. Adamo, C. et al.; J. Chem., Phys., 1999, 110, 6158–6170.
4. Swallow, J., et al., Mater. Horiz., 2020, 7, 236.
5. Fukumoto, M.et al., Adv. Funct. Mater., 2022, 32, 2110832.

Modelling Chemical Interface Damping of Surface Plasmons

Jordan Edwards, Imperial College London

Metallic nanostructures exhibit fascinating optical properties arising from surface plasmons. The properties of surface plasmons can be modified by functionalising the nanostructure with molecular adsorbates. For example, a significant reduction in the surface plasmon propagation length after functionalisation has been

experimentally observed. This phenomenon is known as chemical interface damping (CID). However, the physical origin of CID remains unclear, with two proposed mechanisms being: (1) excitation of electron-hole pairs involving adsorbate orbitals, and (2) electronic scattering by adsorbate-induced dipoles.

To resolve this issue, we perform first-principles density-functional theory calculations for different molecules adsorbed on Au (111) surfaces. We evaluate both the contribution to CID from mechanism (1) and also determine the adsorbate-induced dipoles. We find that mechanism (1) can explain the observed changes in plasmon propagation length, suggesting it is the dominant contributor to CID. These findings offer valuable insights for the design of metallic nanostructures for photocatalysis and plasmonics applications.

Quantum Embedding Methods for Ground States and Excitation Spectra

Basil Ibrahim, King's College London

Mean-field methods such as Hartree-Fock and Density Functional Theory are widely used to model the electronic structure of molecules and materials. While these approaches are computationally efficient, they often struggle to describe systems in which strong interactions between electrons play an important role. More accurate methods exist, but their computational cost grows rapidly with system size, limiting their applicability to realistic materials and complex molecules.

Quantum embedding methods provide a practical route to overcoming this challenge by dividing a system into smaller subsystems, each treated using an accurate many-body calculation while the surrounding environment is described at the mean-field level. The information from these calculations is then combined to describe the properties of the full system. Well known examples include Dynamical Mean-Field Theory (DMFT) and Density Matrix Embedding Theory (DMET). This talk will introduce the basic ideas behind these approaches and discuss a method that connects the two frameworks. Applications to molecules and solids will be presented, including calculations of ground state properties and excitation spectra.

Examination of the electronic conductivity of multi-heme-protein junctions using a multiscale simulation methodology

Andras Petho, University College London

Proteins offer huge promises for bioelectronic applications, including the development of sensors and bio-wires. These compounds offer a variety of structures with several examples of proteins taking part in electron transfer processes. Despite this our understanding of their conductive behaviour is incomplete. The full characterization of the conductive behaviour of these compounds could greatly advance our efforts to design novel bioelectronic devices.

Multi-heme cytochromes, proteins with covalently bonded heme cofactors are a group of compounds showing great promise in such applications as their conductivity rivals that of organic semi-conductors Compared to an average protein the conductivity of MHCs is a magnitude higher, however the reasons behind this increase of conductivity are poorly understood.

This contribution showcases a study during which we have computationally examined a set of six MHC-gold junctions, to gain insight into the molecular behaviour behind their electronic conductivity. In the scope of the initial project, we have investigated 81 full junction structures as well as a further 18 artificial systems where we have removed the segments thought most crucial for conduction to investigate their roles. Two extensions of the investigation will also be introduced. First, we looked at how hydration changes the electronic conductivity of junctions then another extension was done where the electronic properties of artificially designed proteins were examined.

Our main findings indicate that we have successfully developed a realistic model to compute the current-voltage response for such junctions, and this indicates the conduction mechanism to be coherent tunnelling. As well as highlighting the importance of the secondary structure of the protein in governing the conductance.

Furthermore, we have found that the conductivity strongly depends on the density of states of the proteins with larger systems supporting stronger currents. These indicate that using MHCs as bio-wires could be a promising avenue in bioelectronic applications.

The Role of Electron Correlations in Chirality Induced Spin Selectivity of Molecular Junctions

Aadi Konidena, King's College London

Chirality Induced Spin Selectivity (CISS) is an exciting phenomenon where the geometry of helicoid molecules evidently determines the resulting electron spin when a current is driven through the molecule. Despite experimental backing, the details of the primary mechanism that drives spin selection is still not understood. In fact, theoretical simulations based on spin-orbit coupling alone still disagree substantially with experimental data, prompting the investigation into alternate rationales for the observed spin-polarised current. To assess the possible role of the electron-electron correlation effects in current spin polarisation, we study the quantum transport through a molecular junction with Hubbard interactions added on each site of a helical molecule alongside the spin-orbit coupling. We employ the Non-Equilibrium Green's Function formalism and Feynman diagram technique to account for the Hubbard interactions within the Second Born approximation. To calculate the spin current as a function of the temperature and the applied bias, our treatment goes beyond the simple Landauer approach and incorporates the Hubbard self-energies in the equation for the full current.

ComProScanner: Multi-agent-based composition-property data extraction framework

Aritra Roy, London South Bank University

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

Coupled Trajectory Quantum-Classical Molecular Dynamics for Charge Transport in Organic Semiconductors

Aaron Dines, University College London

Accurately simulating charge and energy transfer is essential for predicting and designing technologies such as solar cells, batteries, and light-emitting diodes. However, these processes depend on coupled electron–nuclear dynamics that break the Born–Oppenheimer approximation. To model such behaviour computationally, a range of quantum-classical nonadiabatic molecular dynamics (QCNAMD) methods have been developed, in which nuclei are treated classically while charge carriers evolve quantum mechanically. These methods may be considered a direct generalisation of traditional molecular dynamics, wherein the electronic dynamics is also directly propagated. Despite the successes of QCNAMD methods, the exact form of the quantum–classical coupling remains an open problem.

A promising approach is coupled-trajectory mixed quantum-classical dynamics (CTMQC), which derives this coupling from a rigorous connection to the full quantum-mechanical description. Recent algorithmic developments have also made CTMQC sufficiently robust for large-scale simulations. In this work, we combine CTMQC with the fragment orbital basis (FOB) framework for parameterising electronic structure in organic semiconductors, enabling the first CTMQC simulations of frontier-orbital-mediated charge transfer in a nanoscale naphthalene crystal at 300 K.

We show that the resulting methodology, termed FOB-CTMQC, reproduces the key successes of the established FOB surface-hopping (FOB-SH) framework, while additionally revealing transport mechanisms inaccessible to surface hopping, including prolonged charge delocalisation events. We further demonstrate that variants of FOB-CTMQC are basis-independent and therefore insensitive to the trivial crossing problem that affects surface hopping in systems with high electronic state densities. Finally, we discuss possible extensions to CTMQC, including schemes that naturally produce local wavefunction collapse onto nearby molecular sites.

Machine learning defect thermodynamics for high-throughput dopability screening

Savyasanchi Aggarwal, University College London

Dopants are intentional impurities introduced into a semiconductor lattice to tune the functional properties of a material – whether by affecting its electronic, physical or structural properties. The key advantage of doping is its low synthetic cost, but it is often difficult to predict whether the concentration of dopants is high enough to tune the material in the required manner. A common bottleneck for this is the relative formation energy of intrinsic defects in the system – these will often outcompete any dopants if the formation energy is low enough, making the system 'undopable'. Thus, a reliable metric for determining the tunability of a material for any commercial application is the presence of any 'doping windows', where the formation energy of intrinsic defects is high enough to not outcompete dopants.

In theoretical chemistry, this window is traditionally evaluated using density functional theory (DFT) using a high level of theory to accurately define electronic structures. Despite the powerful accuracy of this technique, it is fundamentally limited by its high computational cost, which necessitates the use of several approximations and chemically biased structure searching methodologies to evaluate the formation energies of intrinsic defects. However, these methods still prove far too slow for effective high-throughput searching, which is certainly necessary for navigating the vast chemical space of possible dopants and hosts.

In this talk, I will describe the work I have performed throughout my PhD to develop a defects-specific machine learning interatomic potential (MLIP) with global charge definition to screen for dopability in semiconductors in a rapid, high-throughput manner. Notably, I will showcase how my methodology maintains near-DFT accuracy in predicting defect thermodynamics in several wide-bandgap oxides, and how this approach can be extended to capture meaningful intricate chemistry in defects at a fraction of the traditional computational costs.

Sampling point defect distributions in amorphous HfO_2 using machine learning interatomic potentials

Isaac Mackley, University College London

Point defects in amorphous oxide materials are of significant technological interest, yet they present a fundamental challenge for computational modelling. In crystalline materials, high symmetry limits the number of inequivalent defect sites, making systematic DFT studies straightforward. In amorphous systems this symmetry is absent: every defect site occupies a distinct local environment, meaning that a statistically meaningful description of defect properties requires sampling across large numbers of configurations. This makes direct DFT studies - particularly with hybrid functionals - extremely expensive and raises a further question of whether a given set of calculations is representative of the true distribution.

Machine learning interatomic potentials (MLIPs) offer a potential route to addressing this challenge, combining near-DFT accuracy with computational costs orders of magnitude lower than DFT. However, training MLIPs for defect systems in amorphous materials is non-trivial: the model must generalise across a highly diverse landscape of local environments, and generating sufficient high-quality training data itself carries a significant DFT cost.

In this work we use nitrogen (N) interstitials in amorphous HfO_2 (a-HfO_2) as a test case to explore MLIP-based workflows for defect modelling in amorphous systems. a-HfO_2 is a technologically important high-κ dielectric material used in CMOS and ReRAM devices, and N is a relevant dopant species. We fine-tune the MACE-OMAT

foundation model using CP2K DFT calculations, systematically comparing training data strategies ranging from static snapshots to geometry optimisation trajectories. We find that trajectory-based training data, combined with Bader charge filtering to control defect charge state, yields a model capable of correctly relaxing N interstitial configurations across diverse amorphous environments. We discuss the trade-offs between training data cost and model quality, and the prospects for applying this workflow to generate formation energy distributions and charge transition level statistics for defects in amorphous systems more broadly.

Data-driven methods for discovering high-efficiency photovoltaics

Matthew Walker, University College London

The explosion in compute power and the availability of large chemical databases has prompted a wave of data-driven materials discovery routines for a range of properties and applications, of which photovoltaics (PVs) are but one. However, campaigns seeking to find materials to reduce the planet's carbon footprint should be mindful of their own carbon footprint.

We outline a series of PV discovery workflows that combine traditional computational chemistry calculations and machine learning (ML) surrogate models and establish the Pareto front for balancing the accuracy of such workflows against their carbon cost. We then consider more lightweight approaches: deep learning models require large datasets to tune their thousands or millions of parameters, while statistical methods with heavy inductive bias built-in (available due to our knowledge of chemistry and physics) with few parameters can make use of small datasets. Such datasets are often all that is available for high-fidelity data and/or niche properties. We use the Fused Gromov-Wasserstein distance, a measure that uses optimal transport to find the difference between graphs (which we can use to represent materials), to guide a similarity-driven PV discovery campaign. Starting from materials with high PV efficiency, we screen materials databases for 'nearby' structures and find a number of previously unexplored high-efficiency materials, validated with hybrid density functional theory.

We demonstrate that methods that are less data- and energy-hungry still have their place in functional materials discovery.

Field-Driven Molecular Response with Perturbed Neural Network Potentials

Kit Joll, University College London

Perturbed neural network potentials (PNNPs) provide a route to machine-learning molecular dynamics under externally applied static and time-dependent fields. By learning the response of a system to external perturbations, PNNPs make it possible to access field-dependent dynamical, spectroscopic, and transport properties at a fraction of the cost of direct first-principles simulation.

In this talk, I will introduce the PNNP method and demonstrate its application to liquid water and aqueous electrolyte solutions. For liquid water, I will show how static and oscillating electric fields can be used to compute dielectric response, water reorientation lifetimes, and infrared spectra. I will then present applications to aqueous cation solutions, where non-equilibrium molecular dynamics under static fields allows ionic conductivities to be calculated directly. Together, these results highlight PNNPs as a powerful framework for studying molecular response in complex condensed-phase systems, particularly when long trajectories and explicit field-driven dynamics are essential.

Plenary Speaker Abstracts

Emergent Collective Phenomena in Low-Dimensional Materials

Giorgia Fugallo, Ecole Normale Supérieure, CNRS Researcher, Associate Editor for Computational Materials Science, and past winner at the TYC Student Day (2011)

In low-dimensional materials, reduced dielectric screening, quantum confinement, restricted scattering phase space, and enhanced many-body effects profoundly affect lattice dynamics, electronic excitations, and light–matter interactions, enabling physical regimes that are absent in conventional three-dimensional systems.
In this talk, I will discuss how these effects reshape thermal and optical response in 2D materials, driving the breakdown of conventional bulk descriptions such as Fourier transport and standard three-dimensional exciton models. Particular emphasis will be placed on collective phenomena associated with strong phonon and light–matter interactions, including phonon hydrodynamics and room-temperature second sound, together with exciton and phonon superradiance in the crossover from monolayer to bulk systems, opening new perspectives for nanoscale photonics and energy-efficient thermal management.

Biography: Giorgia Fugallo is a CNRS researcher at the Physics Department of the École Normale Supérieure (ENS) in Paris. She received her PhD in Physics from King's College London in 2012. Before joining CNRS in 2017, she held postdoctoral positions at Sorbonne University and at the École Polytechnique Fédérale de Lausanne (EPFL) and was awarded the EDF–École Polytechnique Research Fellowship in Renewable Energies.

Her research focuses on first-principles and multiscale modelling of materials for energy applications, with particular emphasis on 2D and van der Waals materials. Her work explores anharmonic effects, thermal transport, and vibrational and electronic spectroscopies, including the development of first-principles methods for phonon transport implemented in the *thermal2* package of the open-source Quantum ESPRESSO suite.

She served on the CNRS National Committee, is a member of the steering committee of the European Theoretical Spectroscopy Facility (ETSF), serves as Associate Editor of Computational Materials Science, and was the winner of the TYC Student Day in 2011.

[1] G. Fugallo et al., Nano Lett. 14, 6109 (2014).
[2] A. Cepellotti et al., Nat. Commun. 6, 6400 (2015).
[4] G. Fugallo et al., Phys. Rev. B 98, 184307 (2018).
[4] C. Elias et al., Phys. Rev. Lett. 127, 137401 (2021).
[5] G. Cassabois et al., Phys. Rev. Research 4, L032040 (2022).
[6] G. Cassabois et al., Phys. Rev. X 12, 011057 (2022).
[7] M. Poulos et al. Phys. Rev. B 110, 075434 (2024)
[8] T. Ferre et al. J. Phys. Chem. C 129, 5511 (2025)

Accelerating materials design with AI emulators and generators

Claudio Zeni, Senior Researcher at Microsoft Research Cambridge

Materials design is a challenging and time-consuming process that requires exploring a vast and complex chemical space. To accelerate this process, we present MatterSim and MatterGen, two novel models that can emulate and propose novel materials with desired properties.

MatterSim is a machine learning model actively trained from large-scale first-principles computations for efficient atomistic simulations at first-principles level and accurate prediction of materials' properties across the periodic table and across a wide range of temperatures and pressures. MatterGen is an atomistic generative model that can propose novel and stable materials across the periodic table. Furthermore, the model can be fine-tuned to conditionally generate stable, novel materials with desired chemistry, symmetry, as well as mechanical, electronic, and magnetic properties.

These models unlock the large-scale discovery, exploration, and simulation of novel crystalline materials under a wide range of thermodynamic conditions, and open new possibilities for computational materials design.

Biography: Claudio Zeni is a senior researcher and project lead at Microsoft Research within the AI for science initiative. He applies AI to materials design and simulation and is interested in ways to bridge the gap between computational and experimental materials science via AI.

Claudio achieved his Ph.D. in computational physics at Kings' College London in 2020 and then worked as a researcher at the International School for Advanced Studies in Trieste before joining Microsoft in 2022.

Posters

1	Polaron Formation and Dynamics in Amorphous SiO_2 Gianmarco Biagi, University College London
2	Developing a data-driven atomistic model for asphalt aging Rebecca Driver, King's College London
3	Data driven design of organic mixed conductors Kate Ellis, King's College London
4	The good, the bad, and the ugly of atomistic learning for 'clusters-to-bulk' generalization Mikolaj Gawkowski, University College London
5	Applications of Generative AI to Constitutively Active Orphan GPCRs Azaan Hafeez, Queen Mary University of London
6	Non-adiabatic dynamics simulation of charge generation in organic solar cells Filip Ivanovic, University College London
7	Computational approaches to eumelanin structure elucidation Klára Jašková, King's College London
8	Towards "Ab-initio" Lattice Free Energies of Molecular Crystals with Fine-Tuned Foundation Models and Normalising Flows Harveen Kaur, University College London
9	Modelling excited state absorption of metal-organic frameworks (MOFs) using cluster and periodic approaches Selin Kilic, University College London
10	Reasoning-Guided Optical Chemical Structure Recognition for Ambiguous Polymer and Markush Representations Ruikang Li, King's College London
11	Energy conservation in coupled-trajectory mixed quantum classical dynamics Peter Ng, University College London
12	Sticky Metals: An Investigation into Diffuse Interfaces and Adhesion Ray Omer, University College London
13	Examination of the electronic conductivity of Multi-heme-protein junctions using a multiscale simulation methodology Andras Petho, University College London
14	Understanding Altermagnetic Behaviour in Cobalt Difluoride Laura Poysti, University College London
15	Controlling the phase behaviour of ultraconfined water via bilayer graphene stacking Yixuan Pu, University College London
16	The Spin-MInt Algorithm: An Accurate and Symplectic Propagator for the Spin-Mapping Representation in Nonadiabatic Dynamics James Rampton, University College London
17	Atomistic model structures and electron transfer properties of Nickel bis(1,2-dithiolene)-based nanoribbons linked to electronic conduction in cable bacteria Ollie Russell, University College London
18	Tailoring Polarisation in Ferroelectric $PbTiO_3$/$SrRuO_3$ and $PbTiO_3$–$BaTiO_3$ Heterostructures: A DFT Investigation of Hydrogen Adsorption, Strain and Oxygen Vacancies Nisrine Sakaki, London South Bank University
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20	Free Energy Perturbation Enables Accurate Prediction of Bisphenol Binding to Estrogen Receptors Rianne van Diest, University College London
21	Hydrodynamic Backflow for Easing the Fermion Sign in Finite-Temperature Electron Path Integral Simulations Ingvars Vitenburgs, Imperial College London
22	Data-driven methods for discovering high-efficiency photovoltaics Matthew Walker, University College London

23	Coarse-grained Modelling of Chiral Octahedral Porous Organic Cages Crystal Structures Tingting Wang, Imperial College London
24	Complex ordering phenomena in the multiferroic quadruple perovskite BiMn$_7$O$_{12}$ from ab-initio density functional theory Chung Ping Xu, University College London