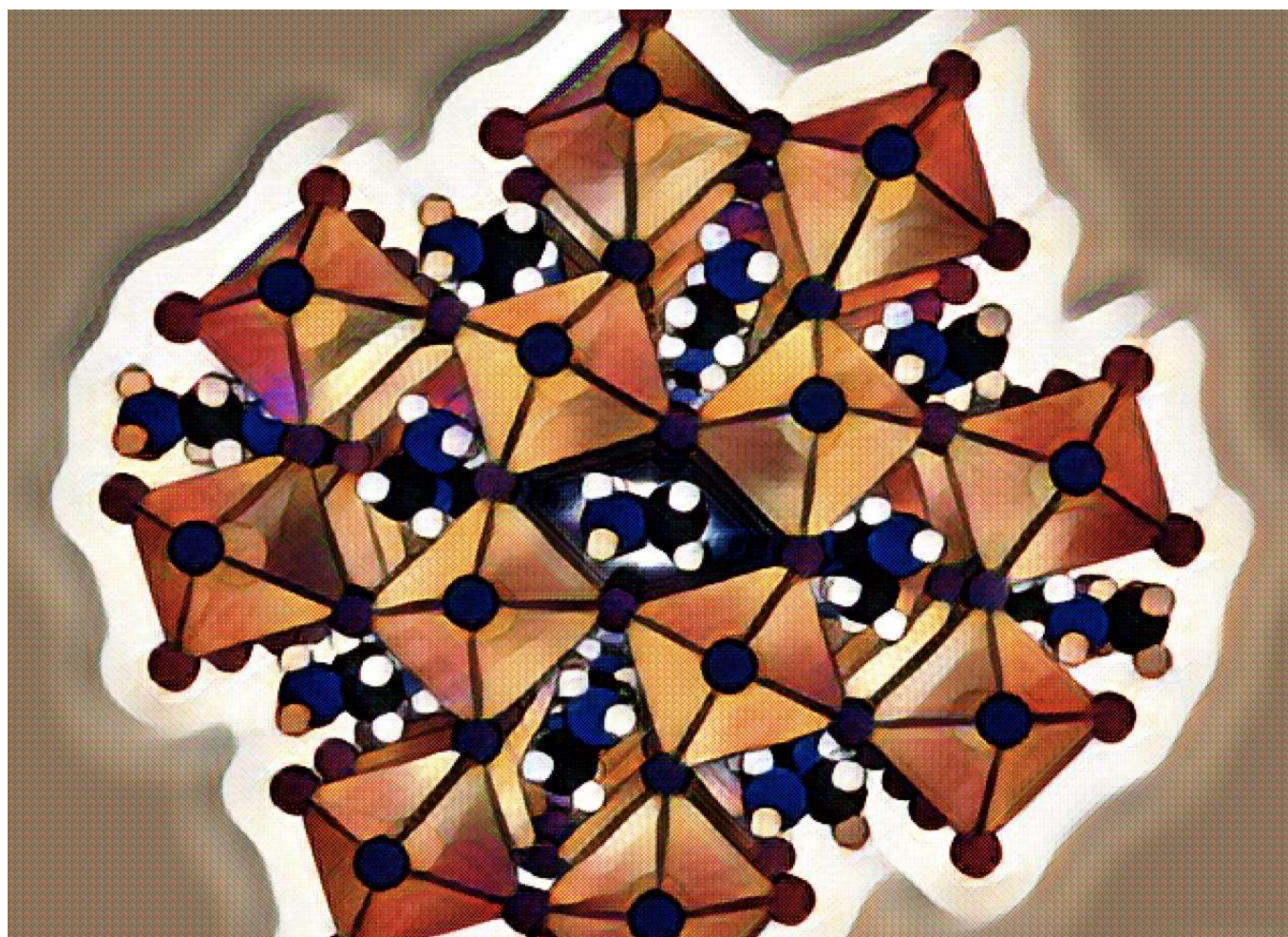


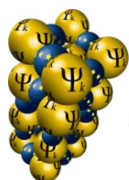


Thomas Young Center 7th Energy Workshop

Programme & Abstracts

24th July – 26th July 2024 – Imperial College London, White City MSRH (Room: B10)

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**APL Machine
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Contents

TYC 7 th Energy Organising Committee.....	2
Conference Contributors.....	2
Chairs	2
Poster Judges	2
Programme.....	3
Wednesday 14 December	3
Thursday 15 December	4 - 5
Friday 16 December	6
Abstracts – Invited and Contributed talks	7
Matthew Rosseinsky.....	7
Volker Deringer	7
Becky Greenaway	7
Robert Palgrave	8
Shubham Vishnoi.....	8
Anthony Onwuli.....	9
Pascal Friederich.....	9
Hanna Tuerk	10
Simao Joao.....	10
Alexander Bagger	10
Juliana Morbec	11
Olivier Henrotte.....	12
Jeremy Frey	12
Tom Penfold	12
Jose Recatala Gomez	13
Alex Ganose.....	13
Mahika Luthra	13
Jaqui Cole	14
Seungwu Han.....	14
Venkat Kapil.....	14
Federico Hernandez	15
Tian Xie	16
Kedar Hippalgaonkar	16
Posters.....	18



TYC 7th Energy Organising Committee

Keith Butler, University College London
Clotilde Cucinotta, Imperial College London
Johannes Lischner, Imperial College London
Alin Marin Elena, Science & Technology Facilities Council (STFC)
Amel Mazari, Imperial College London
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Programme

Wednesday afternoon (July 24): Automation and acceleration

Chair: Aron Walsh, Imperial College London

- | | |
|--------|---|
| 1.30pm | Registration open |
| 1.50pm | Welcome |
| 2.00pm | Matthew Rosseinsky (University of Liverpool)
Discovery synthesis of inorganic functional materials in the digital age |
| 2.30pm | Volker Deringer (University of Oxford)
Machine-learning-driven advances in modelling battery materials on the atomic scale |
| 3.00pm | Coffee break |
| 3.30pm | Becky Greenaway (Imperial College London)
High-Throughput Approaches for the Discovery of Organic Materials |
| 4.00pm | Robert Palgrave (University College London)
Challenges in high-throughput inorganic material prediction and autonomous synthesis |
| 4.30pm | Shubham Vishnoi (Limerick University)
High-throughput Computational Screening of Sustainable, Eco-friendly Crystal Piezoelectrics |
| 4.45pm | Anthony Onwuli (Imperial College London)
Expanding materials embeddings for more expressive machine learning models |
| 5.00pm | Discussion (led by Aron Walsh) |
| 5.30pm | Poster session & Prizes (Room: G23/24) |

Programme

Thursday morning (July 25): From atoms to devices

Chair: Martijn Zwijnenburg, University College London

- | | |
|---------|--|
| 9.30am | Pascal Friederich (KIT)
Machine Learning for Simulation, Understanding, and Design of Molecules and Materials |
| 10.00am | Hanna Tuerk (EPFL)
Unlocking the Potential of Lithium Thiophosphate: Searching Chemical Moieties that Determine Surface Reactivity |
| 10.15am | Simao Joao (Imperial College London)
Computational nanoparticle screening for efficient plasmo-catalysis |
| 10.30am | Coffee break |
| 11.00am | Alexander Bagger (DTU)
Data-driven symbiosis between computations & experiments for electrochemical reactions |
| 11.30am | Juliana Morbec (University of Keele)
Designing organic/2D heterostructures for photovoltaic applications |
| 11.45am | Olivier Henrotte (Munich)
Energizing materials with sunlight |
| 12:15pm | Discussion (led by Martijn Zwijnenburg) |
| 12.45pm | Lunch |

Programme

Thursday afternoon: Data for large-scale facilities and benchmarks

Chair: Keith Butler, University College London

- | | |
|--------|---|
| 2.00pm | Jeremy Frey (STFC)
The Physical Sciences Data Infrastructure (PSDI) |
| 2.30pm | Tom Penfold (Newcastle University)
Deep Neural Networks for X-ray Spectroscopy: Hero or Zero? |
| 3.00pm | Jose Recatala Gomez (NTU)
Accelerated solid-state synthesis of functional inorganic materials |
| 3.15pm | Coffee break |
| 3.45pm | Alex Ganose (Imperial College London)
Computational materials discovery in the age of automation |
| 4.15pm | Mahika Luthra (Aarhus University)
Screening of Oxide Catalysts using Machine Learning Foundation Models |
| 4.30pm | Jaqui Cole (University of Cambridge)
Data platforms for materials scientists |
| 5.00pm | Discussion (led by Keith Butler) |

Programme

Friday morning (July 26): From force fields to generative models

Chair: Clotilde Cucinotta, Imperial College London

- | | |
|---------|--|
| 9.30am | Seungwu Han (Seoul University)
Application of pretrained machine learning force fields to energy materials |
| 10.00am | Venkat Kapil (University College London)
Towards full quantum first-principles simulations via machine learning |
| 10.15am | Federico Hernandez (University of Bristol)
Quantum and machine learning photodynamics of solid-state materials for energy applications |
| 10.30am | Coffee break |
| 11.00am | Tian Xie (Microsoft)
MatterGen: a generative model for inorganic materials design |
| 11.30am | Kedar Hippalgaonkar (NTU)
Property-directed generative design and experimental validation of inorganic crystals |
| 12.00pm | Discussion (led by Clotilde Cucinotta) |
| 12.30pm | Prize winners announced |
| 12.40pm | End of Conference |

Abstracts – Invited & Contributed talks

Discovery synthesis of inorganic functional materials in the digital age

Matthew Rosseinsky – University of Liverpool

Machine-learning-driven advances in modelling battery materials on the atomic scale

Volker Deringer – University of Oxford

High-Throughput Approaches for the Discovery of Organic Materials

Becky Greenaway – Imperial College London

Dynamic covalent chemistry (DCvC) is a powerful tool for assembling complex organic molecules, such as organic cages, which can be synthesised using a range of enabling technologies, including flow chemistry, mechanochemistry, and high-throughput automation, enabling both their scale-up and the ability to screen a broad synthetic space. They can also be processed into different phases of porous organic materials with potential applications in carbon capture and energy-intensive molecular separations, including crystalline porous solids with interconnected pore networks, amorphous glasses, and porous liquids, or used as building blocks in more complex supramolecular assemblies such as metal-organic cages or frameworks, or mechanically-interlocked catenanes and rotaxanes. However, the targeted design of such molecules can be challenging, especially as the systems become more elaborate, because the reversibility and dynamic nature of DCvC has the potential to form a wide range of different species, making the prediction of the reaction outcome particularly difficult. Traditional experimental approaches, such as making small iterative changes to precursors, trial and error screening of reaction parameters, and relying on serendipitous discovery, are labour intensive and time-consuming. The combination of building blocks possessing varying functionality and topicity, across a range of reaction conditions, creates a chemical space too vast to explore manually on a reasonable timescale. High-throughput automation can be used to rapidly screen a broad synthetic space, and we have previously shown it is particularly effective for organic cages and structurally related porous liquids. However, even with the aid of high-throughput automation, bottlenecks remained in data acquisition and characterisation on an equally high-throughput timescale. In addition, the majority of commercially available automated platforms are prohibitively expensive making adoption in other labs difficult. Here, I will broadly introduce our streamlined high-throughput experimental workflow that makes use of a low-cost, open-source automated platform combined with computer vision and automated data analysis, and supported by computational modelling, to streamline the automated discovery of organic cages. Finally, extension of this workflow for automated porous liquid screening, directed using previous high-throughput data, will be introduced.

Challenges in high-throughput inorganic material prediction and autonomous synthesis

Robert Palgrave – University College London

Materials prediction coupled with autonomous synthesis and characterisation suggests the possibility of closed loop, unsupervised materials discovery. Technological progress has long been marked by deployment of new inorganic materials. Automation that can accelerate rates of materials discovery far beyond those of traditional laboratories might be expected to stimulate advances in many areas of science and technology.

Despite rapid progress in artificial intelligence, robotics, and computational methods, many hurdles remain before autonomous materials discovery becomes a reality. Here, from an experimentalist's point of view, I will discuss some recent successes and failures of autonomous inorganic materials discovery and give an outlook on the challenges still to be overcome.

High-throughput Computational Screening of Sustainable, Eco-friendly Crystal Piezoelectrics

Shubham Vishnoi – University of Limerick

Organic molecular crystals are an emerging class of eco-friendly piezoelectric materials that are both biocompatible and biodegradable enabling their use in Lead-free biomedical applications and smart devices while ensuring eco-friendly production and disposal. The vast majority of organic materials naturally lack a centre of symmetry in their crystal structure, endowing them with piezoelectric properties. In these non-centrosymmetric crystals, a surface charge is generated under an applied force due to ionic displacement. Advances in high-performance computing have facilitated the use of quantum mechanical calculations to predict a variety of electromechanical properties including full piezoelectric tensor of molecular crystals. High-throughput density functional theory (DFT) based crystal screening employs computational methods to rapidly assess the electronic and structural properties of numerous crystal structures. Through the implementation of high-throughput screening, we have successfully conducted a comprehensive computational analysis of organic molecular crystals and their predicted electromechanical properties. This effort has resulted in the creation of a large database that can be used as a base for training machine learning models. We highlight the broad range of electromechanical properties amongst the simulated organic crystal dataset, and in particular, the high number of crystals that have a naturally occurring longitudinal d_{33} constant. This longitudinal electromechanical coupling is a prerequisite for several conventional sensing and energy harvesting applications, the presence of which is notably rare amongst the literature on biomolecular crystal piezoelectricity to date. Keywords: organic crystals; piezoelectric materials; quantum mechanical prediction; density functional theory; high-throughput screening.

Expanding materials embeddings for more expressive machine learning models

Anthony Onwuli – Imperial College London

Conventional approaches to structure-agnostic learning in materials science utilise machine-readable representations of the elements (1) (2). These representations are often pooled to form composition-based feature vectors to represent materials. Beyond their utility for property prediction, element representations also have applications for defining the chemical similarity of compounds for structure substitution approaches (3) (4). For incorporating ionic information, descriptors based on oxidation states and electronegativity can be incorporated into element representations. However, to our knowledge, we have not found representations of the ions in the literature. Here, we propose SkipSpecies, a method of learning distributed representations of ions which is an adaptation of SkipAtom, a method for learning distributed representations of atoms (5). Using these ionic representations, we have demonstrated that they can enhance structure-agnostic learning by performing better than element-based representations in predicting the electronic band gap. These ionic representations can offer utility for enhanced ML-assisted compositional screening, structure substitution and doping suggestions which can aid in the discovery and optimisation of novel compounds for energy materials.

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Machine Learning for Simulation, Understanding, and Design of Molecules and Materials

Pascal Friederich- Karlsruhe Institute of Technology

Machine learning can accelerate the screening, design and discovery of new molecules and materials in multiple ways, e.g., by virtually predicting properties of molecules and materials, by extracting hidden relations from large amounts of simulated or experimental data, or even by interfacing machine learning algorithms for autonomous decision-making directly with automated high-throughput experiments. In this talk, I will focus on our research activities on graph neural networks for property prediction [1] and understanding of structure-property relations [2], as well as on the use of machine learning for accelerated atomistic simulations [3,4] and design of materials for energy applications [5].

- [1] Reiser et al., Communications Materials 3 (1) (2022), <https://www.nature.com/articles/s43246-022-00315-6>
[2] Teufel et al., xAI (2023), <https://arxiv.org/abs/2211.13236>
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[5] Wu et al., JACS 2023, <https://pubs.acs.org/doi/full/10.1021/jacs.3c03271>

Unlocking the Potential of Lithium Thiophosphate: Searching Chemical Moieties that Determine Surface Reactivity

Hanna Tuerk- L'École polytechnique fédérale de Lausanne (EPFL)

Lithium thiophosphate (LPS) is a promising solid electrolyte candidate for the next generation of lithium-ion batteries. However, the high reactivity of LPS with common contaminants such as atmospheric water, solvents used for preparation, and common electrode materials hinders commercialisation of the cells. The unknown structure, morphology, and chemical behaviour of LPS's surface prevents strategic solutions to this problem.

Computational nanoparticle screening for efficient plasmo-catalysis

Simao Joao – Imperial College London

Plasmonic nanoparticles offer an attractive avenue for catalysis due to their reactivity and tunability of their plasmonic resonance, and the hot carriers generated from the plasmon's decay offer an additional process that can be leveraged. The nanoparticles' properties can be adjusted to optimise for specific chemical reactions, but predicting the effect of light in chemical reactions requires understanding the role of hot carriers in the catalytic process. Standard electronic structure methods, such as those based on first-principles density-functional theory, cannot be applied to nanoparticles of experimentally relevant sizes. To address this challenge, we use a recently developed approach that combines an atomistic tight-binding description of the nanoparticles with a Chebyshev decomposition of Fermi's golden rule to calculate the rate of hot carrier generation and energetic distribution of electrons. High-throughput computation allows us to compute the properties of many different combination of nanoparticle parameters to find the optimal ones for specific applications. In this talk, we explore the effect of aspect ratio, light frequency, and polarization in Au nanoprisms to find how they can be chosen to optimize the rate of hot electron generation and the rate of hot hole generation in these nanoparticles.

Data-driven symbiosis between computations & experiments for electrochemical reactions

Alexander Bagger- Technical University of Denmark

Electrochemistry holds the promise to be a cornerstone for the sustainable production of fuels and chemicals. However, these catalytic reactions are increasingly complex to understand and hereby also improve. In particular reactions that suffers from selectivity challenges such as CO₂ reduction In this talk, I will discuss how experiments and computational simulations can support each other. I will focus on electrochemical reduction of NO_x, CO₂, N₂, and the combinations. Importantly, all these reactions share a direct competition with hydrogen, and furthermore, several products are formed from each reactant of these reactants. I will give minimalistic models that do not overfit or over interpreting experimental data.

Examples are:

- i) Electrochemical CO₂ reduction show multiple different products depending on metal catalyst [1]. I will show why copper is unique as catalyst with a multiple-carbon product distribution [2]. Following I will discuss data analytics on copper facets to steer the product distribution [3].
- ii) ii) Electrochemical NO_x reduction, also multiple products are formed; N₂O, N₂ and NH₃[4]. Several catalyst enable reductions to ammonia amongst them copper [5] and recently also Co and Fe based catalysts close to their reduction potential [6].
- iii) iii) Electrochemical N₂ reduction to ammonia (NH₃) at ambient conditions is burgeoning [7-8]. Most interesting in aqueous there is not a “copper” catalyst [9]. While in nonaqueous, the univocally working system is a Li-mediate system [10]. For this system, I will show that varying multiple experimental parameters display similar performance characteristics [11] and I will discuss systems beyond lithium.

Finally, I will discuss how one can use these insights to establish predictive schemes for products beyond the typical reduction reaction products, hereunder synthesis of urea [12].

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Designing organic/2D heterostructures for photovoltaic applications.

Juliana Morbec- Keele University

Combining two-dimensional (2D) materials with organic materials can be very attractive for applications that require flexibility and where size and weight are important parameters to be considered, such as in wearable, portable and mobile applications. Organic materials usually exhibit excellent optical absorption efficiency and photo- and temperature-induced conformational changes, while 2D materials often show relatively high carrier mobility, superior mechanical flexibility, and tuneable electronic and optical properties. Combining both systems can stabilize the organic materials and lead to heterostructures with both high carrier mobility and high optical absorption efficiency, which is promising for solar energy conversion. In this work we investigate, by means of density-functional-theory calculations, heterostructures composed of organic molecules (for example, pentacene and azulene) and transition metal dichalcogenides (TMD) for application in photovoltaic devices. We examine the interaction between the molecules and monolayer TMDs as well as the band alignment of the heterostructures, considering effects of the molecular coverage, rotation, and dielectric screening [1,2].

[1] Interaction between pentacene molecules and monolayer transition metal dichalcogenides, E. Black, P. Kratzer and J. M. Morbec. Phys. Chem. Chem. Phys. 25, 29444 (2023).

[2] Effect of molecular rotation and concentration on the adsorption of pentacene molecules on two-dimensional monolayer transition metal dichalcogenides, E. Black and J. M. Morbec, submitted (2023).

Energising materials with sunlight

Olivier Henrotte (Munich)

This talk will primarily focus on the strategic manipulation of light using plasmonic and photonic structures to harness, convert, and store solar energy. I will delve into our recent experimental research efforts, aimed at understanding the intricate interplay between these structures and sunlight, with a focus on optimizing their efficiency for energy utilization. I will present a series of studies that seek to establish correlations between plasmonic/photonic photocatalytic activity and factors such as reactivity, temperature, and field at the nanoscale. By uncovering synergies between plasmonic and photonic materials, we aim to unlock their full potential across various applications, particularly in solar energy conversion and storage. Through these endeavors, we aspire to contribute to the development of sustainable technologies that address the urgent global need for clean and renewable energy sources.

The Physical Sciences Data Infrastructure (PSDI)

Jeremy Frey – STFC

The data infrastructure to support the physical sciences lags well behind that of the life sciences and the growing importance of data led approaches making use of AI and particularly machine learning (ML), has highlighted the need for proper support for the collection, curation, dissemination of data in context and with good provenance in machine as well as human readable forms. I will describe the PSDI initiative and how it is and plans to help the community address these needs.

Deep Neural Networks for X-ray Spectroscopy: Hero or Zero?

Tom Penfold- Newcastle University

X-ray spectroscopy delivers strong impact across the physical and biological sciences by providing end users with highly detailed information about the electronic and geometric structure of matter. To decode this information in challenging cases, e.g., in operando catalysts, batteries, and temporally evolving systems [1], advanced theoretical calculations are necessary. The complexity and resource requirements often render these out of reach for end users, and therefore, the data are often not interpreted exhaustively, leaving a wealth of valuable information unexploited. In this talk, I will discuss our recent progress applying machine learning to the prediction and interpretation of X-ray spectroscopy [2,3]. This DNN can predict transition metal K-edge X-ray absorption near-edge structure spectra in less than a second with no input beyond geometric information about the local environment of the absorption site. We predict peak positions with sub-eV accuracy and peak intensities with errors over an order of magnitude smaller than the spectral variations that the model is engineered to capture. I will also discuss its extension to other absorption edges, interpret the performance of the network and demonstrate how the uncertainty arising from predictions can be estimated. Finally, I will highlight areas on which future developments should focus.

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Accelerated solid-state synthesis of functional inorganic materials.

Jose Recatala Gomez- Nanyang Technological University

Materials discovery lays the foundation for many technological advancements. The discovery progress is slow, with an estimated 20 years between discovery and commercialization. This process is even slower for materials that require solid-state synthesis due their sluggish diffusion coefficients and long diffusion distances. Here, we present 6S, a self-sintered scalable solid-state synthesis technique, a one-pot technique that produces densified phase-pure polycrystalline materials in a high-throughput manner at 1-10g/min. We demonstrate 6S's versatility across various inorganic functional materials, including the synthesis and thermoelectric evaluation of AgSbTe₂ and Bi-Sb-Te alloys, which show competitive thermoelectric figure-of-merit. Likewise, we synthesized iron-cobalt alloys, compounds for the state-of-the-art conversion of CO₂ to C₅+ products using thermal catalysis. Moving forward, we envision 6S not only as an effective method for synthesizing current materials but also as a platform for discovering new materials.

Computational materials discovery in the age of automation

Alex Ganose- Imperial College London

Screening of Oxide Catalysts using Machine Learning Foundation Models

Mahika Luthra – Aarhus University

Metal oxides are promising catalysts for the hydrogenation of CO₂ into valuable chemicals like methanol. Among these, solid solutions of ZrO₂ are particularly interesting due to the easy availability of Zr and long-term stability during methanol production. Experimental studies have demonstrated that doping ZrO₂ with other metals enhances catalytic activity, attributed to the synergistic effects between Zr and dopants.[1] In our study, we focus on predicting the methanol-producing capabilities of these doped ZrO₂ solutions using density functional theory in combination with machine learning foundation models. We employ CHGNet,[2] a pre-trained universal neural network potential tailored for charge-informed atomistic modelling as the foundational model for screening these materials. We test the capabilities of CHGNet for accelerating common tasks in catalyst screening such as structure optimization of the catalyst material, prediction of oxygen vacancy formation energies, and the computation of binding energies and barriers of elementary reaction steps such as H₂ dissociation and CO₂ hydrogenation. We find that while the pre-trained model lacks predictive accuracy for energies, particularly for more complex adsorbates, it can, in many cases accelerate computational workflows as a pre-optimizer of structure. Finally, we discuss the potential for fine-tuning the model to increase its accuracy for screening ZrO₂-based catalysts. Our work lays the foundation for employing machine learning foundation models to develop kinetic models for the catalytic activity of metal oxides within electrochemical and thermal conversion of CO₂, which can further enhance our understanding of catalytic mechanisms to guide the synthesis of novel materials.

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Data platforms for materials scientists

Jaqui Cole- University of Cambridge

Application of pretrained machine learning force fields to energy materials

Seungwu Han- Seoul National University

Recently, message-passing graph neural network interatomic potentials (GNN-IPs), particularly those with equivariant representations such as NequIP, have attracted significant attention due to their data efficiency and high accuracy. Moreover, the atomic embedding vector in GNN-IPs allows for training over large datasets with diverse chemistry, resulting in pretrained, general-purpose machine learning force fields. In this presentation, we introduce the development of an efficient parallelization scheme compatible with GNN-IPs and its implementation into a package named SevenNet (Scalable EquiVariance-Enabled Neural NETwork), which is based on the NequIP architecture. We then pre-train SevenNet with a vast dataset from the Materials Project (dubbed ‘SevenNet-0’) and demonstrate its out-of-distribution generalization capabilities. We subsequently apply SevenNet-0 to investigate electrolytes in lithium batteries, such as screening organic molecules in liquid electrolytes and identifying new solid-state electrolytes.

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Towards full quantum first-principles simulations via machine learning

Venkat Kapil – University College London

Computational chemistry and material science hinges on the precision and efficiency of first-principles simulations. Ideally, these simulations should incorporate the quantum nature of all electrons and nuclei, achieving predictive accuracy across areas from protein folding, drug design, and catalysis to nanoscale thermodynamics and quantum materials. Traditional “full quantum” simulations are, however, computationally prohibitive. This presentation introduces a modern first principles framework that significantly reduces these costs while maintaining high fidelity. Our method leverages physics-based machine learning to estimate the system’s Born-Oppenheimer potential energy surface and other essential electronic quantum effects, such as polarization and polarisability. Demonstrating its efficacy, we predict hitherto unfeasible first-principles phase diagrams of nanoscale systems [1] and relative stabilities of molecular crystal polymorphs [2].

Further, we address the challenge of modelling nuclear motion by mapping quantum dynamics to an effective classical correction akin to effective potentials by Feynman and Hibbs [3]. Our work translates quantum nuclear motion to simple classical molecular dynamics. To showcase our method’s capability, we predict vibrational spectra of bulk and interfacial aqueous phases, achieving quantitative agreement with experiments for the first time [4]. Our model offers a path for

comprehensive quantum simulations, combining accuracy with the ease of prevalent classical methods.

References

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Quantum and machine learning photodynamics of solid-state materials for energy applications

Federico Hernandez – University of Bristol

Light-activated phenomena underpin applications in energy materials. This process takes place in the condensed phase, where the environment has an active role by either restricting the motions of the excited molecules or directly participating in the main excited mechanisms. A full understanding of these phenomena at the atomic level is required to optimize quantum efficiencies and aid the design of new materials with tailored properties. Excited state dynamics provides an insightful picture of light-activated processes at the intra- and intermolecular levels. However, computational studies of photophysics and photochemistry in the solid state is extremely challenging because of the substantial computational cost of high-fidelity calculations of chromophore excited-state dynamics in periodic systems. We developed a new approach combining a multiscale QM/QM' electrostatic embedding scheme with nonadiabatic molecular dynamics to model the photochemistry and photophysics of molecular crystals. We use this scheme to train machine learning (ML) models to solve the photodynamics of systems that are intractable at the QM level, enabling fully atomistic excited-state dynamics for the solid state with multiconfigurational quantum mechanical calculations.

We test our approach studying: 1) The photochemistry of crystalline norbornadiene/quadracycline (NBD/QC) derivative systems, one of the top candidates for Molecular solar thermal (MOST) applications, also known as solar thermal fuels. Solid-state MOST materials are particularly interesting as they can offer maximised energy densities and do not require encapsulation for applications as their liquid counterparts. However, the study of solid-state MOST systems is limited due to the added complexity arising from the solid environment. We modelled the excited state dynamics from photon absorption predicting lifetimes and the corresponding quantum yields of the primary and degradation photoproducts formation with high level of accuracy. 2) We combine the high-level electrostatic embedding multiscale multiconfigurational approach and ML photodynamics to understand singlet fission dynamics in pentacene crystals. We identified two competing SF channels underpinning the high efficiency of SF in pentacene crystal with our simulations. Our ML-photodynamics enables the resolution of the elusive interplay between electronic structure and vibrational relations in the SF dynamics, highlighting the essential role of intermolecular vibrations in generating the multi-excitonic state.

MatterGen: a generative model for inorganic materials design

Tian Xie- Microsoft

The design of functional materials with desired properties is essential in driving technological advances in areas like energy storage, catalysis, and carbon capture. Traditionally, materials design is achieved by screening a large database of known materials and filtering down candidates based on the application. Generative models provide a new paradigm for materials design by directly generating entirely novel materials given desired property constraints. In this talk, we present MatterGen, a generative model that generates stable, diverse inorganic materials across the periodic table and can further be fine-tuned to steer the generation towards a broad range of property constraints. To enable this, we introduce a new diffusion-based generative process that produces crystalline structures by gradually refining atom types, coordinates, and the periodic lattice. We further introduce adapter modules to enable fine-tuning towards any given property constraints with a labelled dataset. Compared to prior generative models, structures produced by MatterGen are more than twice as likely to be novel and stable, and more than 15 times closer to the local energy minimum. After fine-tuning, MatterGen successfully generates stable, novel materials with desired chemistry, symmetry, as well as mechanical, electronic, and magnetic properties. Finally, we demonstrate multi-property materials design capabilities by proposing structures that have both high magnetic density and a chemical composition with low supply-chain risk. We believe that the quality of generated materials and the breadth of MatterGen's capabilities represent a major advancement towards creating a universal generative model for materials design.

Property-directed generative design and experimental validation of inorganic crystals

Kedar Hippalgaonkar- Nanyang Technological University

A combination of AI, high-throughput experiments (robotics) and high-performance simulations can be used to accelerated materials development. I will first start by describing our efforts at lab-to-tech, where our technologies have been instrumental in successful formulation discovery, optimization as well as commercialisation (both with industry partners and through our startup, Xinterra Inc.) In order to leverage these tools further, the ultimate goal is to achieve AI-driven materials discovery. Here, an important principle is that structure determines property. Therefore, property-driven generative design, driven by machine learning, critically requires understanding of the structure of materials. A deep understanding of crystal structures and their symmetries is essential for accurate generative design.

Thus, the development of symmetry-aware generative models becomes critical to ensure property-directed learning branches. Further, generated crystal structures require validation, both computationally and experimentally. After validation, the challenge is the experimental

synthesis of these materials, which must be paired with data-driven characterization techniques to assess their properties. This is challenging due to the lack of a general method to rapidly synthesize and (optimally) dope bulk materials. In our work, I will discuss the how all of these come together and how we address a key bottleneck by the invention of a rapid self-sintered solid-state synthesis technique (tested on GeTe, Copper, Silver Antimony Telluride), achieving phase-pure crystalline materials synthesized in the milligram scale in as little as 15 seconds. This accelerates the solid-state reaction process by a factor of >100 relative to the traditional route of mix-and-bake.

Posters:

1	Rafia Ahmad	Advancing Sustainable Energy Solutions: Novel Materials for CO ₂ Valorisation and Catalyst Understanding
2	Ohud Alshammari	Electronic Conductance and Thermopower of Cross-Conjugated and Skipped-Conjugated Molecules in Single-Molecule Junctions
3	Chantal Baer	A computational study of the chemical stability and ionic conductivity of Li-metal/Li-argyrodite interfaces
4	Amit Chaudhari	Machine learning the DFT+U projectors to model polarons in correlated energy materials
5	Wenxuan Cai	Modelling core electron binding energy on metal oxide surfaces
6	Jordan Edwards	Chemical interface damping of surface plasmon polaritons
7	Lucas Garcia Verga	Data-driven Exploration of Adsorption Site Ensembles on Mixed Metal Oxides
8	Filip Ivanovic	Thermoelectric transport in crystalline organic semiconductors is driven by space and temperature-dependent electronic disorder
9	Konstantin Jakob	Universally Accurate or Specifically Inadequate? Stress-Testing General Purpose Machine Learning Interatomic Potentials
10	Kit Joll	Machine learning the electric field response of condensed phase systems using perturbed neural network potentials
11	Se Hun Joo	Expediting Cathode Material Discoveries through Ab Initio Random Structure Searches and Machine-Learned Interatomic Potentials
12	Jisu Jung	Off-lattice kinetic Monte Carlo simulation of Pt ₃ Co nanoparticle degradation using machine-learned potential
13	Chaiyawat Kaewmeechai	Theoretical modelling of charge trapping in crystalline and amorphous Ga ₂ O ₃
14	Luuk Kempen	Data-efficient modelling of metal–oxide interfaces using global optimization and machine learning
15	Xiliang Lian	Understanding fluoride ion diffusion in BaSnF ₄ through machine learning molecular dynamics
16	Xia Liang	Machine Learning Optimisation and Structural Dynamics of Hybrid Halide Perovskites
17	Alice Meng	Automated High-Throughput Exploration of Stable and Active Iridium Mixed Oxides for Green Hydrogen Production
18	Harpriya Minhas	Exploring the Hidden Influence of Cationic ns ² Lone Pair Electrons on Thermal Conductivity in Pnictogen Chalcogenides through Machine Learning
19	Irea Mosquera Lois	Machine learning point defect reconstructions
20	Ilias-Panagiotis Oikonomou	Identifying point defects in liquid-phase exfoliated PtSe ₂
21	Hyunsoo Park	A multi-modal pre-training Transformer for universal transfer learning in porous materials.
22	András Pethő	Investigating conductive properties of single-heme cytochrome
23	Joe Pitfield	Towards Universal applicability of Universal interatomic potentials
24	María Eugenia Sandoval Salinas	Spin control of conjugated systems in inert matrices
25	Huseyin Sener Sen	Atomistic Simulations of Interfaces within All-Solid-State Batteries: A special case of Lithium Thiophosphates
26	Seung-Jae Shin	Microscopic Origin of Electrochemical Capacitance in two-dimensional Metal Organic Frameworks
27	Ned Taylor	RAFFLE: Materials Interface Structure Prediction

28	Matthew Walker	Machine Learning for Discovery of New Polar Photovoltaics
29	Shirui Wang	Computational insights into emerging chalcogenide perovskite photovoltaics
30	Xinwei Wang	Predicting Solar Cell Efficiency from First Principles
31	Ruiqi Wu	Tilt-induced charge localisation in phosphide antiperovskite photovoltaics
32	Chengcheng Xiao	Brillouin zone sampling in ONETEP
33	Jiwen Yu	Static and molecular dynamics of density functional tight binding (DFTB) simulations for brucite carbon dioxide storage