1. Structure-performance behaviour of multilayer capacitors for sustainable electrocaloric cooling

Neil Mathur (Materials Science and Metallurgy), Siân Dutton (Physics)

Devices that exploit electrocaloric (EC) cooling can achieve high efficiency values and be readily miniaturized without a concomitant increase in price or operational complexity, creating vast opportunities for both scientific advancements and technological applicability, e.g. in the microelectronics or automotive industries.

Working at the forefront of EC device performance, our group research electrocaloric materials, devices and performance-evaluation methods. We aim to improve ceramic and polymer EC materials, where electrically driven phase transitions result in large temperature changes, by deepening our understanding of the relationship between structure, operating conditions, and performance.

Anyone taking this project will be encouraged by the dynamic and supportive research group to develop and verify their own ideas, choose whether to introduce theory or computer modelling in combination with the experimental work, and coauthor any resulting publications. Experimental work could involve a range of techniques that include bespoke calorimetry and infra-red imaging. Theory could involve the Landau free energy formalism. Computer modelling could be employed to study heat transfer in experimental systems.

2. In-situ additive manufacture of ODS steel for nuclear applications

Matteo Seita (Engineering), David Collins (Materials Science and Metallurgy)

Next generation fusion and fission reactors require a combination of neutron irradiation, temperature and corrosion resistance unavailable from current commercial alloys. Oxide dispersion strengthened (ODS) alloys have long been suggested as a potential solution to these environmental problems. Current ODS steels are produced by mechanical alloying of yttria (Y) and steel powders in order to dissolve the yttria throughout the steel in a fine dispersion. This process is prohibitively expensive for commercial application due to the long times required for mechanical alloying and the small batches of powder produced. Furthermore, joining of these alloys is also difficult, as conventional welding techniques destroy the desired microstructure. Finally, forming of ODS is also complicated as the typical higher strength means that the material is harder to form following manufacture.

The proposed project looks to simplify the approach by utilizing Y-containing steel powder and additive manufacturing. By maintaining a controlled low-oxygen atmosphere, the Y in the powder will preferentially oxidise during printing, producing the ceramic precipitates required for dispersion strengthening. This concept has previously been shown to work using vacuum plasma spraying; however, it was not determined whether the size and dispersion of these precipitates were appropriate for classification as an ODS steel. It is expected that the fine resolution of 3D printing will provide a higher level of control to the process to achieve the desired microstructure.

3. AI-Guided Discovery of Reticular Materials for Carbon Capture and Photocatalysis

Markus Kraft (Chemical Engineering and Biotechnology), Manish Chhowalla (Department of Materials Science and Metallurgy)

Advanced materials for catalysis and carbon capture are pivotal to improving the efficiency and sustainability of energy production. In carbon capture and catalysis, materials based on reticular chemistry, where molecular building blocks are assembled to create precise and tuneable geometric structures, have demonstrated exceptional potential. Recently, our group has developed a knowledge-engineering platform to systematically map the immediate chemical space of reticular metal–organic polyhedra (MOPs), which has allowed for the identification of structurally feasible, yet-unsynthesised candidates [1, 2].

This project will expand the platform's capabilities to explore broader regions of chemical space and will focus on developing machine learning algorithms and AI agents to propose novel complexes for carbon capture and photocatalysis. Through close collaboration with experimental partners at the Cambridge Centre for Advanced Research and Education in Singapore (CARES), promising materials identified by the AI-driven pipeline will be synthesised, tested, and validated experimentally, creating a dynamic feedback loop to continually refine the computational predictions.

The candidate will contribute to an interdisciplinary team and work at the interface of artificial intelligence, chemistry, and materials science. This project is an excellent opportunity for candidates to develop skills in advanced programming, machine learning methods, large-language models, and computational modelling.

[1] J. Am. Chem. Soc., 2022, 144, 26, 11713–11728

[2] twa: The World Avatar Python package for dynamic knowledge graphs and its application in reticular chemistry, preprint, 2025. https://como.ceb.cam.ac.uk/preprints/335

4. Exploring porous carbon materials for CO_2 capture and reduction using atomistic simulations and NMR

Christoph Schran (Physics), Alex Forse (Chemistry)

This project focuses on the atomistic-level understanding of porous carbon materials for carbon dioxide (CO_2) capture and electrochemical CO_2 reduction, two critical technologies in the fight against climate change. Porous carbons are promising materials due to their tunable pore structure, chemical stability, and low cost, but their performance is closely tied to the complex interplay between local environment, surface chemistry, and confined fluid structure. This project combines advanced atomistic simulations with nuclear magnetic resonance (NMR) spectroscopy techniques to uncover these relationships.

We will employ a range of molecular modelling techniques, using modern advances in machine learning potentials and enhanced sampling, to study the structure and dynamics of confined CO_2 and water mixtures inside functionalised carbon pores. Special emphasis will be placed on understanding how pore size, shape, and surface functionalities affect CO_2 solubility, diffusion, and reaction pathways at the atomic scale.

In close collaboration with Alex Forse's group, the project will also involve the calculation of NMR observables to enable direct comparison with experimental data, providing a powerful link between theory and experiment. The goal is to build a robust and predictive framework for designing porous carbons with optimised properties for CO_2 capture and conversion. This project is part of the FAST (Frontiers in Atomistic Simulation Techniques) group at the Cavendish Laboratory, which develops cutting-edge simulation methods to study aqueous systems, catalysis, and interfaces. The project provides an excellent opportunity to work at the interface of materials modelling, spectroscopy, and sustainable chemistry and will involve direct links to experiment.

5. Neutron Imaging and NMR spectroscopy to understand impact of water adsorption on sorbents for direct air capture of CO_2

Alexander Forse (Chemistry), Sylvia Britto (ISIS Neutron and Muon Source)

The proposed PhD project aims to advance Direct Air Capture (DAC) technology by investigating how water influences CO_2 capture in hydroxide- and carbonate-functionalized sorbent materials. DAC is a promising negative emissions strategy that extracts CO_2 directly from the atmosphere, but its large-scale deployment depends on developing efficient, low-energy, and stable sorbents. Water vapor in the atmosphere plays a complex role in DAC, potentially enhancing or hindering CO_2 uptake depending on humidity levels and material properties. Preliminary data from the Forse Group show that increasing humidity can both activate additional CO_2 capture modes and trigger material degradation over time.

To better understand these phenomena, the project will develop an in-situ neutron imaging setup capable of visualizing water adsorption and distribution in sorbents under real DAC conditions. Neutron imaging, which is highly sensitive to hydrogen, will be used to explore three core objectives: (1) mapping the interplay between water and CO_2 adsorption under varying humidity to determine cooperative or competitive interactions, (2) assessing the uniformity of sorbent functionalization, which impacts performance, and (3) identifying water-induced degradation pathways that reduce CO_2 capture capacity.

By correlating neutron imaging results with complementary in-situ NMR spectroscopy, this project aims to deliver a detailed understanding of water–CO_2 interactions in DAC sorbents. These insights will inform the design of next-generation materials with improved efficiency and durability, contributing to scalable and cost-effective carbon removal solutions.

6. Seed layers for lithium nucleation in anode-free batteries: In-situ NMR and SECCM study

Svetlana Menkin (Chemistry), Clare Grey (Chemistry)

Lithium-anode-free batteries (LAFB) comprise a lithium-ion cathode and a current collector, the cathode consisting of the lithium source. The metal is then plated on the current collector during charging. These batteries present a significant advantage due to their higher energy density, ease of production and improved sustainability, i.e., eliminating graphite and minimising the use of lithium metal. However, the premature failure of metal and AFBs impedes their commercialisation.
The PhD project aims to understand the role of lithium nucleation seed layers on lithium electrodeposition to realise practical AFBs. Seed layers, pre-coated lithium, carbon and zinc, typically produce higher cycling efficiency. Understanding how these layers improve cyclability and affect the heterogeneity of the interface reactions will facilitate more efficient and sustainable development of LAFBs.

The research will employ an interdisciplinary approach, combining in-situ NMR and scanning electrochemical cell microscopy (SECCM) to measure the lithium nucleation and growth, active material loss, and charge transport across the metal-electrolyte interface to explore how conducting coatings and custom battery formation procedures affect lithium nucleation and battery cyclability. In-situ NMR methods, developed in the Grey group, allow lithium and sodium to be tracked while transported during battery cycling. Here, in-situ NMR will track lithium metal formation, dissolution and corrosion rate while plating on different nucleation layers. The Menkin group developed SECCM methods for monitoring the charge transport across the metal-electrolyte interface. SECCM will be used for electrochemical mapping of ‘hot spots’ on the surface and the underlying localised electrochemistry that cannot be detected via methods typically used in the field. Atomic force microscopy (AFM) will be used for the characterisation of the morphology, mechanical and electrochemical properties of the developed seed layers. The AFM work will be done in collaboration with PARK Systems.

7. Next-gen nanoparticle-based looping catalysts for precisely tuned chemical potential of oxidising energy materials

Ewa Marek (Chemical Engineering and Biotechnology), Ljiljana Fruk (Chemical Engineering and Biotechnology)

Our vision is to develop a new class of catalysts, comprising metal particles of Au, Ag, and Au–Ag alloys, and a reducible oxide as support for catalytic oxidation reactions operating under chemical looping conditions. This approach avoids the use of gaseous O_2 and instead relies on lattice oxygen from the reducible support, offering major safety advantages while enabling precise control of oxygen delivery during reaction.

Our goal is to better understand and exploit the interface between noble metal nanoparticles and redox-active perovskite supports, in particular $SrFeO_{3-\delta}$. Previous work has shown that supporting Ag nanoparticles on this oxide enhances oxygen release, both the rate and the level of final conversion of $SrFeO_{3-\delta}$ —features essential in chemical looping. By exploring Au and alloyed Ag and Au nanoparticles, we aim to further tune the redox behaviour, enhance catalytic activity, and stabilise the nanoparticle structure under operating conditions.

A key focus is enabling the direct, selective oxidation of propylene—a long-standing holy grail of heterogeneous catalysis. The project will combine nanoparticle synthesis, in-situ characterisation, and high-throughput testing to identify promising material combinations. A locally trained AI-based model will then be used to establish design rules for redox-active catalysts, paving the way for safer, more selective, and more flexible oxidation technologies.

8. New materials and new device architectures for organic solar cells

Richard Friend (Physics), Hugo Bronstein (Chemistry)

This project focuses on the use of spin-radical organic semiconductor molecules called P3TTM. This work arises from a collaboration between the synthetic chemistry team of Hugo Bronstein in the Yusuf Hamied Department of Chemistry and the semiconductor physics team led by Richard Friend in the Department of Physics. We have developed this class of molecules to give very efficient luminescence, as exploited in organic LEDs. However recent work in our groups shows that they can also function as efficient photoconductors [1] and this opens up a completely new set of designs for molecules and for devices. The existing designs for organic solar cells require interfaces between electron donors and acceptors to generate separated electrons and holes, and suffer from losses due to electron-hole recombination to spin triplet excitons. Our new designs using spin radical molecules avoid both of these issues.

The overall project requires design and synthesis of new spin-radical materials and new design, fabrication and measurement of photovoltaic diodes. There is scope for projects ranging from chemical synthesis through to semiconductor physics.

[1] Li, B., Murto, P., Chowdhury, R. et al. 'Intrinsic intermolecular photoinduced charge separation in organic radical semiconductors', Nat. Mater. (2025). DOI : 10.1038/s41563-025-02362-z

9. Automated synthesis of metal-organic framework materials

Shijing Sun (Materials Science and Metallurgy), Alex Forse (Cemistry)

This project will focus on developing an automated synthesis platform for metal organic frameworks with controlled thermal and mechanical properties.

Metal organic Frameworks have exceptional tune-ability as nanoporous materials and their thermomechanical properties are key for applications as varied as gas storage (where adsorption can strain and heat the MOF), catalysis, and thermoelectric generators. The student will work with a synthesis robot and implement an AI agent to autonomously optimise precursor compositions and processing conditions to achieve targeted thermomechanical properties. Advanced spectroscopy tools will be developed and used for rapid material characterisation and feedback, enabling closed-loop decision-making.

Through this interdisciplinary work, the student will gain hands-on experience in materials chemistry, automation, and machine learning, helping to accelerate the discovery of next-generation energy materials for optoelectronic applications.

10. Extending champion efficiencies in disordered solar cells through machine learning for theory and experiment

Seán Kavanagh (Chemistry), Shijing Sun (Materials Science and Metallurgy)

Cadmium Telluride (CdTe) is the most commercially successful thin-film photovoltaic (PV) solar cell technology, representing a leading candidate for large-scale and sustainable renewable energy production. Champion CdTe devices achieve high solar-to-electricity conversion efficiencies of 23.1% through anion mixing, partially replacing Tellurium with Selenium to passivate defect states and boost carrier lifetimes. Both the atomic origin of increased carrier lifetimes and optimal synthesis strategies remain unknown, however. Modelling defect behaviour in disordered (mixed) systems has remained an intractable challenge due to combinatorial explosion of local configurations, while anion-mixing protocols have been primarily guided by trial-and-error.
This project will employ state-of-the-art machine-learning (ML) approaches to understand the impact of anion mixing on defect properties in this crucial energy material, predict optimal thin-film design strategies and aid their experimental realisation. Defect characterisation will employ computational chemistry tools, ML interatomic potentials (MLIPs) along with Density Functional Theory, to achieve the requisite accuracy and computational efficiency for direct modelling of defect processes in mixed systems. Materials design tools – interpretable ML, computer vision and potentially robotic automation – will be used to analyse experimental datasets and, in combination with atomistic insights, determine optimal synthesis conditions for mixing ratios, grading, heterogeneity etc, to maximise efficiency.

This project employs a cross-disciplinary approach to materials design, using ML techniques but in diverse settings and implementations. Along with answering key questions regarding defect chemistry and achievable efficiencies in this crucial energy technology, this project will establish methodologies for modelling defects in disordered materials, which represent the state-of-the-art across several energy applications – including thermoelectric and photocatalysts.

11. Real-Time Terahertz Sensing for Enhanced Quality Control in Lithium-Ion Battery Electrode Manufacturing

Axel Zeitler (CEB), Michael De Volder (Engineering)

This project aims to develop an advanced terahertz pulsed imaging (TPI) sensor for real-time in-line electrode porosity and thickness monitoring during the calendaring stage of lithium-ion battery (Li-ion) manufacturing. As the demand for higher energy density, longer cycle life, and improved safety in Li-ion batteries continues to rise, significant research has focused on optimising electrode chemistry. However, much less attention has been paid to understanding how manufacturing processes, especially mechanical steps like calendaring, impact the final product's microstructure and performance. These steps play a crucial role in determining key attributes of the battery, such as its durability, performance efficiency, and susceptibility to failure modes like delamination or cracking over time. The calendaring process, which compresses electrode material onto the current collector, significantly influences the porosity and uniformity of the electrode layer. These factors are critical to the battery's long-term performance, impacting ion transport, electrical conductivity, and overall efficiency. Uncontrolled porosity or thickness can lead to uneven stress distribution and performance degradation, making it essential to implement robust, real-time monitoring systems.

In this project, we build upon our recent success in developing terahertz radiation-based methods for measuring the thickness and porosity of powder compacts in other industries, such as pharmaceuticals and automotive manufacturing. Terahertz radiation, with its ability to penetrate non-conductive materials like polymers and ceramics, is well-suited for this application. By adapting this technology specifically for Li-ion battery electrodes, we aim to provide a non-destructive, real-time method to optimise electrode properties during production.

The project will focus on several key innovations. First, we will adapt the measurement system to a transfection geometry, enabling simultaneous measurement of both porosity and thickness. Additionally, we will ensure the technique is compatible with various electrode chemistries and develop a robust platform for integration into the battery calendaring process. Ultimately, this system will provide manufacturers with unprecedented insight into their electrode structure, helping to improve quality control and enhance the performance and reliability of Li-ion batteries. In parallel to the process sensing work, we will investigate the impact of repeated charge/discharge cycles on the porosity and other microstructural changes of the batteries using a combination of in situ terahertz spectroscopy and other characterisation methods such as X-ray microtomography.

12. Crossbar arrays for in-memory computing

Markus Hellenbrand (Materials Science and Metallurgy), Andrew Flewitt (Electrical Engineering)

Artificial intelligence (AI) and Machine Learning applications are experiencing a vast and rapid growth and will affect all areas of our lives. So far, however, they are being implemented in conventional computing architecture, which is not optimised for such applications. Consequently, it will require novel approaches to computing and the underlying materials to make AI sustainable, and among the most promising are neuromorphic computing (or in-memory computing) and resistive switching (RS).

At the University of Cambridge, we developed a new class of industry-friendly resistive switching materials, ‘amorphous nanocomposites’, which demonstrate superior electrical RS performance. The functionality is provided by the unique amorphous nanocomposite structure of the material enabling a fine control of oxygen vacancy concentrations and their transport within the material. Currently, development is at the materials and devices stage. To unlock their full potential, they need to be integrated into circuits, beginning with ‘crossbar arrays’, i.e. a matrix of interconnected devices.

In this project, the student will develop industry-friendly fabrication processes for such crossbar arrays for the most promising switching materials. This will include transfer of exploratory material to industry-friendly deposition tools, development of crossbar layouts and fabrication, and demonstration of experimental image classification directly in hardware, i.e. beyond common software-based approaches. This has the potential for huge energy savings compared with conventional approaches, and will unlock applications from ultra-low-power edge AI to massive-scale data centres.

13. Photoelectrochemical cells with high-drive voltage for generation of green chemical feedstocks

Sam Stranks (Chemical Engineering and Biotechnology), Erwin Reisner (Chemistry)

Green multicarbon C_{2+} products (e.g., ethylene, n-propanol) have high energy density and value. Photoelectrochemical (PECs) cells photo-energise electrons from sunlight to drive chemical processes with suitable catalysts. State-of-the-art PECs with high drive voltage use III-Vs in multijunctions, yet are cost-prohibitive. Promising demonstrations have used solution-processed halide perovskites as photoelectrodes in unassisted water splitting, but the photoabsorbers are susceptible to corrosion. Solar-to-chemical (STC) efficiency has remained <1%. No photoelectrode system has simultaneously met high solar-to-fuel efficiencies, great PEC stability, large photovoltage, and low cost.

Here, we will process thin-film multi-junction halide perovskite photo-electrodes with sufficiently high drive voltages to realise efficient CO_2 reduction to ethylene in the Stranks Lab. The focus will be on chemically stable photoelectrodes with large voltage (~2-2.5 V). The project will start with photo-absorbers utilised for tandem PV, including low-bandgap Pb/Sn perovskite and Pb-based absorbers, and later stages will include triple junction photovoltaic stacks to reach ~3.5 V. The device development work will be guided by advanced characterisations of the photo-absorber stacks and operating PECs, with ready feedback between these elements. These photoelectrodes will be integrated with suitable catalyst systems for CO_2 upcycling to produce high value organic products in the Reisner Lab.