1. Improving Supercapacitors with Highly Disordered Electrodes

Supervisors: Alexander Forse, Chemistry; Cate Ducati, Materials Science and Metallurgy

High rate electrochemical energy storage is essential to enable sustainable technologies, including the increased use of renewables on the electricity grid as well as electric vehicles. This project will explore supercapacitors, which are energy storage devices with advantages of high power and long cycle lifetimes. This project will tackle the key challenge faced by supercapacitors – their relatively low energy densities compared to batteries.

Traditionally the pore size and surface area of the activated carbon electrodes in supercapacitors have been thought to be the key levers for improving performance. This was challenged by a recent paper from the Forse Group, which found that structural disorder is a key metric for determining energy storage capacities. This project seeks to exploit these findings to design and synthesise improved activated carbon electrodes for supercapacitors.

We will develop new synthesis protocols to obtain high-capacitance activated carbons, which will be screened with rapid spectroscopy experiments. Promising carbons will be tested in supercapacitor energy storage devices, and will be scaled working with our industry partner, a major activated carbon producer. To improve the sustainability of the produced activated carbons, we will explore novel carbon feedstocks including waste materials from the clothing industry, as well as alternative forms of biomass waste.

This project has the potential to discover improved energy storage devices that can enable sustainable technologies.

2. Enhancing Power Density and Longevity in Next-Generation Lithium-Ion Batteries

Supervisors: Michael De Volder, Engineering/IfM; Cate Ducati, Materials Science and Metallurgy

Lithium-ion batteries (LIBs) have emerged as a key technology in the global transition toward net-zero emissions, playing a vital role in powering electric vehicles (EVs) and storing energy from renewable sources such as solar and wind. While LIBs offer high energy density, they are often constrained by their limited power density, leading to longer charging times for EVs and difficulties in meeting peak power demands in applications such as microgrids. A spin-out company from the University of Cambridge (Echion Technologies www.echiontech.com) has developed advanced battery chemistries aimed at overcoming these limitations. This PhD project, sponsored by the company, seeks to further enhance both the power density and overall lifespan of these next-generation batteries. Extending battery life is a crucial factor for sustainability, reducing the frequency of battery replacements and minimizing resource consumption and waste. The research will leverage state-of-the-art material processing techniques and novel characterization methods to gain deeper insights into battery operation and improving its performance. Through a multidisciplinary approach, the project aims to push the boundaries of energy storage performance, accelerating the deployment of sustainable energy systems.

3. Barocaloric liquid crystals for zero-carbon heating and cooling

Supervisors: Xavier Moya, Materials Science and Metallurgy; Alex Forse, Chemistry

Heating and cooling are essential to our lives. We rely on them for comfort in our homes and vehicles, and businesses need heating and cooling for productive workplaces and industrial processes. Up to 50% of the world's CO2 emissions can be attributed to heating and cooling. This is primarily due to heating with combustion of natural gas and cooling with compression of greenhouse gases. However, these current heating and cooling technologies are neither energy efficient nor friendly to the environment.

While there has been quite significant progress on other areas of decarbonisation such as wind and solar power, and the electrification of vehicles, the challenge of decarbonising heating and cooling remains. A completely new approach to the way we heat and cool that is energy efficient and not based on the use of harmful gases is therefore required if we are to reach net zero-carbon emissions.

The aim of the proposed project is to study barocaloric effects in liquid crystals, which have properties between those of conventional liquids and those of solid crystals. Liquid crystals exhibit key ingredients to achieve outstanding barocaloric performance that can match application needs, namely: (i) extremely large (colossal) thermally driven changes in entropy, (ii) very small or zero thermal hysteresis, and (iii) extremely large shifts of their transition temperatures with pressure, which when combined all together in the same material promise pressure-driven thermal changes similar to those observed in commercial refrigerant fluids.

4. Modelling Framework for Amorphous Nanocomposite Oxides

Supervisors: Judith Driscoll, Materials Science and Metallurgy; Bartomeu Monserrat, Materials Science and Metallurgy

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, thus leading to vast and growing energy demands. Consequently, it will require novel approaches to computing and the underlying materials to make AI sustainable, and among the most promising are neuromorphic computing and resistive switching (RS).

At the University of Cambridge, we developed a new class of industry-friendly resistive switching materials, 'amorphous nanocomposites', based on hafnium oxide, 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. The moving oxygen vacancies control the height of an interfacial energy barrier between the oxide and the adjacent electrode and the height of this barrier controls the electrical resistance.

Since it is a new class of material, we are only beginning to understand their properties and potential for energy savings. In this project, the student will make use of density functional theory (DFT) coupled with new machine learning techniques to explore fundamental properties of this new class of resistive switching material to help design similar materials for energy-efficient computing. The modelling work will be carried out in close collaboration with experimental work, i.e., will be correlated with experimental data, to validate the methodology.

5. Terahertz Sensing for Enhanced Quality Control in Lithium-Ion Battery Electrode Manufacturing

Supervisors: Axel Zeitler, Chemical Engineering and Biotechnology; Michael De Volder, Engineering/IfM

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 transflection 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 batteries' porosity and other microstructural changes using a combination of in situ terahertz spectroscopy and other characterisation methods such as X-ray microtomography.

Mass produced thermoelectric generators from CNTs

Supervisors: Stuart Scott, Engineering; James Elliot, Materials Science and Metallurgy

Thermoelectric generators (TEGS) are solid-state devices that generate electrical current when subjected to a temperature gradient. Their primary application is for energy harvesting. TEGS require materials with high electrical conductivity but low thermal conductivity, typically semi-conductors. TEGS using carbon nanotube materials have been demonstrated but have so far used single-wall carbon nanotubes with well-defined electrical properties, namely semi-conducting. Via a CVD process, we have access to large quantities of mass-produced multi-walled carbon nanotubes which comprise a mixture of metallic and semiconducting structures, currently unsuitable for TEGs. Mass production is essential to their adoption in cheap and ubiquitous energy harvesting devices, and so this project will investigate ways to produce more suitable mass-produced structures by (1) altering the CVD process and (2) post-processing of the nanotubes. Finally, TEG devices will be constructed, and their performance will be characterised.

7. Artificial leaves for sustainable chemical synthesis

Supervisors: Erwin Reisner, Chemistry; Sam Stranks, Chemical Engineering and Biotechnology

The conversion of solar energy into chemical energy carriers is an emerging approach toward the sustainable production of green fuels and chemicals for a sustainable future. We have recently developed so-called 'artificial leaves' for the direct conversion of the greenhouse gas CO2 and water into simple energy carriers such as hydrogen, syngas and ethanol – a process that mimics photosynthesis. This PhD project aims to overcome the current bottlenecks of this novel solar-to-fuel technology and enable the synthesis of ideal industrial chemical platform chemicals at high efficiency. The student will develop chemical cascade catalyst systems for CO2 upcycling to produce high value organic products in the Reisner Lab in the Department of Chemistry and assemble high efficiency tandem/triple junction perovskite light absorbers in the Stranks Lab in the Department of Chemical Engineering and Biotechnology. The synergies arising from energy-efficient catalysis and high-performance tandem perovskites will make it possible to produce organic chemicals from CO2 using sunlight. This project therefore develops the fundamental science for a real-world solar technology for the sustainable chemical synthesis of chemical building blocks that are widely being used in the chemical industry to synthesise plastics, liquid fuels, and other organic chemicals such as pharmaceuticals.

Key References

1. Andrei, Reisner et al., Nature, 2022, 608, 518-522.
2. Macpherson, Stranks et al. Nature, 2022, 607, 294-300.
3. Pan, Reisner, Stranks et al. Nature, 2024, 628, 765-770.

8. Programmable Catalysis with Catalytic Capacitors: Repurposing CO2

Supervisors: Tzia Ming Onn, Engineering; Ewa Marek, Chemical Engineering and Biotechnology

Advancements in renewable energy technologies such as solar and wind have made it attractive to utilise electrons to tackle sustainability-related problems and to drive important thermal reactions such as converting carbon dioxide to chemicals and fuels, hydrogen production, and ammonia synthesis. To take advantage of these electrons efficiently, we combined ideas from semiconductors and heterogeneous catalysis to create a platform called the catalytic capacitor. Unlike conventional thermal catalytic systems which rely on dissipated heat as energy sources, this platform is capacitive. It stores electrical charges on the catalytic surface using electric fields, and through voltage modulation, the electron density at the active sites can be toggled to regulate surface chemistry and improve the system's performance. Previous works have demonstrated that this capacitor, which relies on a high-k dielectric layer and graphene, was able to accumulate and deplete charges from the catalytic electrode to affect carbon monoxide, a model system in catalysis. This project intends to expand on that work by exploring the same system with an initial target reaction of carbon dioxide with ethylene to produce useful chemicals. This new platform, if successful, will enable the concept of programmable catalysis, allowing users to switch catalysts on and off and move reaction pathways with the press of a button.

9. Nanoscale Understanding Driving Development of High-performance Halide Perovskite Tandem Solar Cells

Supervisors: Sam Stranks, Chemical Engineering and Biotechnology; Cate Ducati, Materials Science and Metallurgy

Halide perovskites are generating enormous excitement for next-generation solar photovoltaics. The big opportunity is in tandem configurations, where multiple absorber layers are combined to push efficiencies beyond conventional silicon technologies. Here, high efficiency all-perovskite and perovskite/silicon tandem solar cells will be developed using solution and vapour processing methods. The fabricated films and devices will be studied using a range of characterisation techniques, including luminescence mapping and advanced nanoscale electron microscopy characterisation to study the impact of processing routes, additives and passivating interlayers on material properties and hence device performance and stability. This information will loop back into device processing, allowing a unique feedback loop between fundamental properties and device fabrication.

10. Synthesis and characterisation of conjugated materials with intrinsic photo charge-generation

Supervisors: Hugo Bronstein, Chemistry; Akshay Rao, Physics

Organic solar cells are a potential source of sustainable electricity for the future due to their potential scalability, processability and unique form-factors. State-of-the-art devices have surpassed 20% efficiency making them ever more competitive with conventional inorganic based technologies. However, a fundamental obstacle that remains to be overcome is how to overcome the exciton binding energy that is present in these materials as this poses an additional energetic cost. Currently this is done by blending together two different materials: a “donor” and an “acceptor” resulting in high complexity.

We have recently discovered a class of organic materials which do not require this complicated blend of two materials, and instead can directly generate free charges under photoexcitation. This discovery will greatly simplify device architecture and reduce energetic losses and increasing overall efficiency.

This PhD project will aim to further develop these new organic materials which are able to directly and efficiently interconvert light and charges. These materials will result in transformative technologies such as single-material organic solar cells and photocatalysts. The student will be able to explore the full range of exciting science in organic solar cell research including chemical synthesis, optical spectroscopy and device manufacture.

11. Exploiting ML accelerated hot random search to explore complex morphologies

Supervisors: Chris Pickard, Materials Science and Metallurgy; Alex Forse, Chemistry

The ability to predict materials structure from first principles has developed into a key tool for computational materials discovery. With early applications on relatively simple crystal structures of a fixed composition, current ones include the search for novel battery cathodes and superconductors.

Despite this progress, first-principles computational structure prediction, based on quantum mechanical simulation, is limited in the complexity of the materials systems that can be reliably explored, and materials micro- and meso-structure is largely unexplored.

There is revolution underway in the field of computational materials modelling, driven by a new generation of machine learned interatomic potentials (MLIPs). Ephemeral data derived potentials (EDDPs) are a form of MLIP, designed to accelerate random structure search. The acceleration achieved can be immense – up to 100,000 times as many structures can be generated using a given computational resource.

A recent innovation has been to exploit this ML acceleration to integrate a long high temperature annealing step into high throughput Ab Initio Random Structure Searching (AIRSS) – so-called hot-AIRSS. This has been shown to allow vastly more complex materials structures to be explored.

In this project we will investigate the capabilities of hot-AIRSS to generate realistic models of materials systems, for example complex carbon networks that are used in sodium ion batteries and supercapacitors. Our new models will be tested through comparison to experimental results from NMR spectroscopy and pair distribution functional analyses. We will seek to understand the structural basis of the recent discovery of disorder-driven energy storage in nano-porous carbons.

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

Supervisors: 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 researches 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.

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

Supervisors: Svetlana Menkin, Chemistry; Clare Grey, Chemistry; [Third supervisor from another department TBC]

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 microscopy (SECM) 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 SECM methods for monitoring the charge transport across the metal-electrolyte interface. SECM 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.

14. In-operando optical investigation of 2D devices

Supervisors: Giuliana Di Martino, Materials Science and Metallurgy; Stephan Hofmann, Engineering

One of the most promising ultra-low energy electronic devices emerging is resistive switching memory (RRAM) which delivers sustainably-scalable neuromorphic computing capable of reducing energy consumption in IT by >50%. 2D memristors leverage the unique properties of 2D materials, such as atomic thinness, high surface area, and tunable electrical properties, making them particularly useful in emerging fields like neuromorphic computing, memory storage, and flexible electronics.

Hofmann's group explores novel materials, metrology and device architectures and have developed unique ways of engineering materials layer by layer (exfoliation and oxidation), as well as unique structural anistropy, that affect transport processes in memristive switching. Understanding 2D heterostructures and resolving anisotropic formation kinetics down to the monolayer level are critical to developing scalable interfacing solutions and unlocking their application potential in emerging nano-optoelectronics.

The ultra-concentration of light recently achieved by the Di Martino Lab, brought to the development of innovative fast ways to study real-time movement of individual atoms that underpins this new generation of ultra-low energy memory nano-devices, thus overcoming the limitations of traditional investigation techniques and allowing sustainable future IT. The Di Martino Lab is pioneer in innovative and unique optoelectrical characterization tools (ACS Nano (2024), 18, 20412) able to study devices in operando and in ambient condition (Nature Electronics (2020), 3, 687), already allowing to gain understanding in hBN and MoS2 memristive devices (Advanced Materials (2022), 35, 2209968).

In this project we aim to explore fundamental questions on material stability, oxidation and atomic dynamics within 2D devices by using highly localised light.

15. Advanced steels with engineered microstructure for fusion applications

Supervisors: Matteo Seita, Engineering; David Collins, Materials Science and Metallurgy

Nuclear fusion represents a concrete alternative to fossil fuel for generating clean energy to power our society. The viability of this technology, however, depends heavily on the development of metal alloys that can withstand the most extreme environment that can be found on the planet. Plasma-facing materials, for instance, must exhibit good strength and toughness, radiation damage tolerance, high thermal conductivity, and creep resistance up to temperatures as high as 650C. The most promising alloys for this task are reduced-activation ferritic-martensitic (RAFM) steels. However, the limited creep resistance of current RAFM steels prevents their use at temperatures higher than 550C.

In this project, we will explore the creep resistance of RAFM steels with a unique microstructure design. Using additive manufacturing technology, we will engineer these materials with “chiral” grain structure and crystal orientation distribution. Because of the tortuous grain morphology as well as the limited availability of high-diffusivity paths (e.g., grain boundaries), these microstructures are expected to exhibit inherent creep resistance without compromising on strength and toughness. The PhD candidate that will work on this project will synthesize these materials in the Department of Engineering, will run conventional mechanical testing as well as creep tests in the Department of Materials Science and Metallurgy, and will collaborate with UKAEA to assess the material’s response to radiation damage. This is a high risk, high gain project with potentially far-reaching implications for the development of fusion technology in the UK.

16. Photon recycling for efficient light emission

Supervisors: Neil Greenham, Physics; Dominic Wright, Chemistry

Outcoupling of light is crucial to the efficiency of emissive technologies such as light-emitting diodes, down-converting phosphors for displays and agricultural light-shaping films, and even photovoltaics (since the ideal photovoltaic must also be a perfect LED). In a high-index material much of the emitted light is waveguided internally and often lost. This project builds on our recent work on photon recycling (https://doi.org/10.1038/s41467-020-14401-1), where waveguided light is recursively reabsorbed and reemitted in the active layer, giving additional opportunities for outcoupling. This already gives a major efficiency boost in perovskite LEDs, and by maximising radiative efficiency and minimising parasitic absorption could achieve 100% outcoupling (https://doi.org/10.1002/adfm.202411556). We will design, implement and test new structures for photon recycling to approach this goal. Alongside device and optical measurements, modelling will be crucial to drive the project. Standard thin-film optics models fail for absorbing materials, and we will implement new models that work rigorously in this regime. We will couple these models with electrical models for LED operation, to account for variations in radiative efficiency with carrier density at different locations in the device. Beyond LEDs, we will expand our work into luminescent films used to shape the spectrum of light in displays and other applications such as agriculture, again aiming to exploit photon recycling to enhance the emission in the desired direction without the need for strong scattering. Finally, we will assess the role of photon recycling in photovoltaics, where it can significantly boost the open-circuit voltage (https://doi.org/10.1038/s41467-024-48887-w).

17. Alloy Nanostructures for Design of Chemical Looping Catalysts and Production of High Value Chemicals

Supervisors: Ewa Marek, Chemical Engineering and Biotechnology; Ljiljana Fruk, Chemical Engineering and Biotechnology

In chemical looping processes, a solid oxide donates oxygen to reactions, eliminating the need for introducing oxygen required for majority of catalytic processes. By eliminating gaseous oxygen from the reaction setup, chemical looping not only improves the safety of the reactor system but also enables intensification of the reactions beyond the current process limits. However, sourcing oxygen from a solid oxides is not as straightforward as taking O2 directly from air : materials need to be active within required temperature/pressure windows. On the other hand, using oxygen-producing solids has numerous advantages such as the control over the speed and location of the oxygen delivery and more control over the distribution of potential products.

Withing proposed project we aim to design tunaeable oxides by adding nanostructured Au-Ag alloy nanoparticles as catalytic components, and apply them for direct oxidation of propylene. Such a reaction is one of the holy grails of chemical industry as it is a solvent-free process with little to no waste but then little selective against the total combustion.

Recently, we demonstrated that oxygen donation from nonstoichiometric perovskite oxides can be manipulated by contacting the oxide with Ag nanoparticles (broad nm range). We observed that in addition to tuning the reaction, the activity of the oxide has been significantly improved. However, Ag nanoparticles can aggregate upon thermal treatment, which deactivates their interaction with the oxide.

In order to improve the catalytic properties and stability, but also increase the range of activation wavelengths, we aim to develop a library Au-Ag alloys using green strategy recently developed within the team. Our alloy systems can additionally be modified to provide attachment to oxide materials resulting in composite catalyst.

After initial assessment of catalytic system, high throughput chemical looping studies will be performed in collaborator's facility at Imperial College London. The experimental results will be used to train machine learning models, developed to search for highly efficient oxide-catalyst formulations. We will further look into the exact transport pathways of oxygen, employing a unique in-situ high-pressure transmission electron microscopy. Finally, we will explore the plasmonic properties of alloys and their synergistic catalytic effects to fully tailor the generation of oxygen and pave the way to design of selective plasmonic catalysts.