# DEPARTMENT OF MATERIALS

# PART II PROJECTS

# 2023/2024

## UNDERGRADUATE PART II PROJECTS

The project descriptions can also be found at:
www.materials.ox.ac.uk/teaching/part2/pt2newprojects.html

Further projects may be publicised at a later date.

There will be an open afternoon on Wednesday 22nd February with introductory talks on Part II from the Part II Co-ordinator. Attendance at these talks is mandatory for all MS students commencing Part II in Michaelmas Term 2023.

Arrangements regarding supervisor availability is given on the next page.

## Prospective Supervisors:

| Name & Email | Availability |
|---|---|
| Prof David Armstrong | Not available on Wed 22 Feb – please email to make arrangements to discuss next week |
| Prof. Hazel Assender | Will be in her office on Wed 22 Feb - the 4th floor of the ETB, room number 40.03 |
| Dr Paul Bagot | Not available on Wed 22 Feb – will be in his office on Friday 24, at 3pm – the 1st floor of Hume-Rothery, room 20.09. |
| Prof. Simon Benjamin | Please email to make arrangements to discuss |
| Prof. Harish Bhaskaran | Not available on Wed 22 Feb – please email to make arrangements to discuss |
| Prof. Sebastian Bonilla | Will be in his office on Wed 22 Feb - the 3rd floor of the ETB, room number 30.19 |
| Prof. Peter Bruce | Not available on Wed 22 Feb – please email to make arrangements to discuss if you are unable to meet with Dr House |
| Prof. Jan Czernuszka | Will be in his office on Wed 22 Feb, 3pm – 4pm, the 1st floor of 21BR, room 10.15 |
| Prof. Marina Galano | Please email to make arrangements to discuss |
| Dr Jicheng Gong | Please email to make arrangements to discuss (see also availability for Angus Wilkinson below) |
| Prof. Nicole Grobert | Not available on Wed 22 Feb – please email to make arrangements to discuss next week |
| Prof. Chris Grovenor | Will be in the Holder Café from 3pm to 5pm on Wed 22 Feb – happy to discuss projects for which he is co-supervisor |
| Dr Rob House | Will be in his office on Wed 22 Feb - the 1st floor of the Rex Richards building, room number 20.42 |
| Dr Anna Kareer | Please email to make arrangements to discuss (see also availability for Angus Wilkinson below) |
| Dr Enzo Liotti | Based in Begbroke – please contact via email to arrange a meeting either in person or via Teams |
| Prof. Sergio Lozano-Perez | Will be in his office on Wed 22 Feb - the 3rd floor of the Holder building, room number 30.06 |
| Dr Basia Maciejewska | Not available on Wed 22 Feb – please email to make arrangements to discuss next week |
| Prof. James Marrow | Not available on Wed 22 Feb – please email to make arrangements to discuss next week |
| Prof. Michael Moody | Not available on Wed 22 Feb – will be in his office on Friday 24, at 2pm – the 2nd floor of Hume-Rothery, room 30.20. |
| Prof Rebecca Nicholls | Not available on Wed 22 Feb – please email to make arrangements to discuss on Thursday/Friday |
| Prof. Mauro Pasta | Two of Mauro's PGR students will be available to discuss these projects – in the meeting room on the 2nd floor of the Rex Richards building |
| Dr Chris Patrick | Will be in the Rex Richards meeting room on Wed 22 Feb - the 4th floor, room 40.11 |
| Prof. Jason Smith | Not available on Wed 22 Feb - will be in his office on Thurs 23 Feb between 10am and 11am, the 3rd floor of the Parks Road building, room 30.10 |
| Prof. Susie Speller | Will be in the Holder Café from 3pm (for 45mins) on Wed 22 Feb |
| Prof. Richard Todd | Will be in his office on Wed 22 Feb - the 4th floor of the ETB, room number 40.23 |
| Prof. Andrew Watt | Please email to make arrangements to discuss |
| Prof. Rob Weatherup | Will be in his office from 3.30pm on Wed 22 Feb - the 1st floor of the Rex Richards building, room 20.09 |
| Prof. Angus Wilkinson | Not available on Wed 22 Feb – will be in his office on Friday 24, 2pm – 4pm, the 1st floor of 21BR, room 10.19. Alternatively, please email any questions or to arrange a Teams call. |
| Prof. Jonathan Yates | Will be in the Rex Richards meeting room on Wed 22 Feb - the 4th floor, room 40.11 |
| Dr Neil Young | Will be in his office on Wed 22 Feb - the 3rd floor of the Holder building, room number 30.10 |

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## 1. Liquid lithium corrosion of materials for nuclear fusion

**David Armstrong** Co-Supervisor(s): Chris Grovenor

For nuclear fusion to be a commercial reality, reactors must be self-sufficient in tritium. The likely route for tritium production is through the capture of a fusion neutron by a 6Li atom which produces a tritium atom. Liquid breeding use large volumes of flowing liquid Li or Li-Pb alloys to produce tritium, but has the major disadvantage of the corrosive nature of liquid Li. Currently a range of steels, Zr, W and V alloys have been proposed as structural components, but few corrosion tests have been completed.

This project will perform liquid lithium corrosion on alloys of interest to our collaborators in the UK Atomic Energy Authority who are designing the STEP fusion reactor, and some will have protective coatings prepared by sputtering. Samples will be examined using optical and scanning electron microscopy, EBSD and EDX. The aim will be to understand what corrosion products are produced and investigate the effect of different microstructures on corrosion resistance. This understanding will then help inform the engineers designing STEP of the best materials to select.

## 2. A model for radiation-curing of polymers

**Hazel Assender**

We have used various forms of radiation curing to polymerize diacrylate monomers to a solid, crosslinked polymer layer for coatings in functional materials and devices. Experimental data suggest that the degree of cure depends on the amount of radiation, but also the time it is applied and the depth of material. This project will seek to model these data and understand the crosslinking behaviour, and subsequent swelling and mechanical properties of the material. There is scope for practical work to generate more data as required, but the focus of the project will be on the creation of a model to link density of formation of reactive centres (radicals) with the nature of the cross-linked network.

### 3. Microchannel Electrodes for Implantable Neuronal Interfaces

**Hazel Assender**

This project, in collaboration with James FitzGerald, Dept. Surgical Sciences, seeks to develop a structured microchannel polymer that can be used as an interface to receive an array of neuron signals e.g. for prosthetics. The work will involve casting a structured PDMS material and vacuum-depositing metal electrodes in the microchannel structure and electrical testing, **in vitro**, and possible **in vivo** (rat) of the resulting devices. The incorporation of controlled-release drugs (e.g. anti-scarring) into the structure will also be considered.

### 4. Control of diffusion and swelling of hydrogels or elastomers

**Hazel Assender**

Hydrogels and elastomeric materials find multiple applications in medicine, and control of diffusion and swelling of the material, sometimes over extended periods can be important for applications including drug delivery, tissue engineering and to allow recovery following surgical implantation. This project provides the opportunity for an underpinning study into strategies for control of diffusion and swelling in such materials, including in the increasingly complex shapes that might be applied.

### 5. Predicting the performance and usefulness of near-term quantum computers

**Simon Benjamin**

Quantum computer prototypes are reaching the point that they are interesting beyond being physics experiments. For example, in 2019 Google announced a 53 qubit device, which is sufficiently large that no conventional computer can predict its behaviour and in 2022 a IBM boasted a device with over 400 qubits. However, the question of whether such machines can be useful for anything is still undecided; because each elementary operation, or ‘gate’ in the machine is imperfect, with up to 1% noise, the output after many gate operations is very noisy and imperfect. All such devices are called NISQ for Noisy Intermediate Scale Quantum systems.

In order to investigate ways in which such machines can be harnessed, it is valuable to have emulator software – this is software that runs on a conventional computer and accurately models how a quantum computer would behave, including any noise processes. The costs in terms of memory (RAM) and runtime rapidly become impractical as the number of qubits rises past 40, but there is much to be learned by emulating even small systems.

The project will include these themes:

- Understand the key concepts of how we use software to emulate quantum computers (especially the QuEST system that uses either Mathematica or c code as the user interface)
- Understand how quantum algorithms are believed to be superior to conventional algorithms for tasks like predicting the properties of novel materials or chemicals.
- The main part: Investigate whether these quantum algorithms can really work on near-future quantum hardware that suffers from imperfections in all operations. In tackling this, it will likely be useful to talk to experimental teams, both in Oxford and elsewhere, so as to understand the particular problems their prototype hardware has and thus emulate those problems accurately. The concept of quantum error mitigation will likely be key.

This project will involve a considerable amount of computer programming and mathematics, and will suit a student who has previous programming experience and enjoys that kind of task.

### 6. New nanoscale materials for next-generation device engineering

**Harish Bhaskaran**

[Description to follow.]

### 7. Development of novel fabrication techniques for devices

**Harish Bhaskaran**

[Description to follow.]

## 8. The quantum properties of molecular graphenoids

**Lapo Bogani**

Graphene is a material with amazing structural, conducting and mechanical properties. On the other hand, it is still difficult to add one property to it: a magnetic behaviour. This is because graphene is, by itself, diamagnetic. We could recently introduce spin states into synthetic graphene nanostructures by chemical functionalization (Nature 2018) and topological manipulation (Science 2019). On the other hand, one ingredient remains missing: a sizeable spin-orbit coupling, which would allow mixing electronic and spin states so as to create truly multifunctional topological materials. In this project you will investigate our next generation of graphene materials, where metal centres with high spin-obit coupling have been introduced. You will measure the quantum and classical spin properties using advanced pulsed electron paramagnetic resonance techniques, and interpret the results. In this project you will learn the basics of quantum information, advanced pulse techniques for their implementation, and the relevant data treatment. This is a project aimed at a student interested in learning advanced instrumentation, where most of the time will be spent on data acquisition and treatment.

## 9. Optimal Software Interfacing for quantum systems

**Lapo Bogani**

Quantum systems rely on a specific features to achieve performance, and the data treatment poses specific challenges and issues. In this project you will mostly interface with datasets that have already been acquired in order to decipher several of the quantum features of the materials. The project will see the development of dedicated software and will allow learning a variety of languages and tools oftentimes used in large data processing, such as mathematica, matlab, java, python etc... In this project you will push the current limits in how data are modelled and you will need to develop a solid scientific understanding of the underlying phenomena. This is a project designed for a student who wants to improve their informatics and data treatment skills. You will learn how to model large datasets and the challenges associated, and you will need to understand the experimental challenges and the phenomena that are associated with the quantum systems. You will test what characteristics allow for optimal performance, and eventually you will learn the basics for large datasets representation and discussion.

## 10. Tunable Field Effect Devices Using Dielectric Nanolayers

**Sebastian Bonilla** Co-Supervisor(s): Anastasia Soeriyadi

Field effect devices are used in many applications including computing microchips, memories, and optoelectronic devices. We are particularly interested in the solar energy application of such devices. Many well-known dielectric layers contain permanent charges that can be used to manipulate charge carriers inside semiconductors. We have recently developed a process to tune the intensity of these charges on a silicon substrate.

In this project, the student will first learn and reproduce the processing required to create nanolayers with fixed charge. They will then develop a robust method to design the spatial distribution of the nanoscale dielectric layer as well as the intensity of the charges, which can then be integrated into solar cell precursors. The student is expected to have a basic understanding of semiconductor devices. The project involves a hands-on fabrication process in a cleanroom environment followed by electrical and optical measurements. The big aim of the group is in accelerating the transition to clean energy by improving solar cell performance while minimising production costs.

## 11. Metallisation Technology for Next-Generation Photovoltaics

**Sebastian Bonilla**

Solar photovoltaic cells use metal contacts made primarily of screen-printed silver, and in some cell designs the metallisation also requires a transparent conducting film of indium tin oxide. The use of these materials is currently limiting further reductions in cell manufacturing cost, with the metals used contributing as much as one quarter of the cost of the cell. The ongoing trend to reduce the price of solar panels requires the shift towards a metallisation schemes that minimise the use of such expensive or nonabundant materials. This project aims to explore novel contact and metallisation technologies that can address this critical hurdle for the future of solar electricity generation. Silver-free metal to semiconductor contacts will be explored in collaboration with our international partners, and new technologies will be proposed to achieve low-cost manufacturing of efficient metallisation for single and multijunction solar cells.

This project requires hands-on electrical and optical measurements of materials, as well as data processing and analysis. Analytical and electrical characterisation techniques will be used to assess the performance of the metallisation, including advanced nano scale mass-spectroscopy and electrical current transport. The understanding and development from this project will result in improved manufacturing of commercial solar panels, which in turn will help mitigate the devastating consequences of climate change.

## 12. Semiconductor Device Modelling of Tandem Solar Cells

**Sebastian Bonilla**

In order to move to a low-carbon future, and avoid the worst effects of anthropogenic climate change, continuing reductions in the cost of renewable energy are required. Novel tandem photovoltaic devices have emerged as key enabling technology to achieve improvements in efficiency of solar panels. The main aim of this research project is to develop new finite element simulation techniques with the potential aiding the design and boosting the performance of tandems solar cells, overcoming the drawbacks of conventional single junction solar cells. This project will involve the development of finite element based computer models to understand and optimise tandem devices. It will use the understanding from other members of the team working on semiconductor processing to test new material concepts and architectures using computer models. Th student is expected to have a strong background and motivation to use computer simulations, and ideally experience with numerical packages like Python, Matlab, or similar. The developments here can impact the development of next-generation silicon-based photovoltaics, and can result in reductions in the cost and wide deployment of solar energy.

## 13. Environmental switching of gels

**Jan Czernuszka**

Alginates are great mimics for mucus in mammals. They can also be made into gels relatively simply. This project will aim to use alternative cations to crosslink the gels and provide pH switches.

## 14. Cleaning up dirty lakes, rivers and seas.

**Jan Czernuszka**

Hydroxy apatite is a scavenger of cations and anions and short chain organics. This project will look at how different waste products can be either adsorbed or incorporated into the lattice.

## 15. Fabrication of Oxide based ceramic matrix nano-composites for creep applications at 1100°C

**Marina Galano** Co-Supervisor(s): Richard Todd, Talha Pirzada

The proposed Part II project aims to develop the creep resistance properties of existing oxide-oxide ceramic matrix composite (CMC) materials. The project will involve introducing nanoparticles to the developed CMC slurry system to enhance its creep properties, with the aim of producing light-weight, high-temperature, creep-resistant aeroengine components. The project will include engineering a manufacturing process to produce stable, homogeneous dispersions of nanoparticles in a ceramic slurry. CMC sample panels will be produced using this process and then passed through a test matrix to quantify their mechanical properties. This would include room temperature and high temperature flexural and creep testing, and characterisation of the samples produced (XRT and DVC).

The objectives of this project are

i) to produce a TRL 3 process for producing stable, homogeneous ceramic slurry containing nano and micro scale particles, and

ii) Achieve and verify improvement in creep resistance through nano-engineering of the CMC matrix, microstructure.

## 16. Optimising the manufacturing process of Oxide based Ceramic Matrix Composites for heat shields in gas turbine and rocket engines

**Marina Galano** Co-Supervisor(s): James Marrow, Talha Pirzada

The UK’s first prepreg line is being established to produce oxide based prepreg that will be used to manufacture ceramic matrix composite components for gas turbine seals and rocket engine heat shields. Testing needs to be done in order to ensure that the components perform adequately in service conditions.

This project will involve mechanical and morphological characterization of the material system at room and high temperature. This will include room temperature and high temperature flexural and creep testing, and characterization of the samples produced (XRT and DVC). The failure mechanism under load will be identified using 3D strain analysis. Creep tests will be carried out, in tandem with X-ray tomography, on these material systems in order to optimise the layup strategies.
The objectives of this project are

i) to quantify the mechanical properties of the material system produced in the UK at RT and at 1100°C
ii) to understand the failure mechanisms of these material systems.

## 17. Miniaturised high-cycle fatigue testing of crack initiation and short crack growth in aero-engine materials

**Jicheng Gong** Co-Supervisor(s): Angus Wilkinson

Fatigue is the most pervasive failure mode across the industrial sectors. Our group developed a novel fatigue testing technique that can assess a small volume of material at an extremely fast rate (400 and 20 KHz, respectively), enabling a high cycle fatigue (HCF) test in hours in contrast to months using the conventional approach.

This project will use these new techniques to investigate HCF crack initiation and short crack growth in aero-engine materials (Ti, Ni or steel). Meso-scale cantilevers will machined in metallic foils by means of a micro-laser and mechanically assessed using high-frequency fatigue rig. The deflection of a cantilever is measured by a laser calibration system. A set of SN curves will be achieved with respect to the stress ratio and testing frequency. Intermittent and post-mortem analysis by SEM and EBSD will be conducted to characterise the fracture surface. Finite element model will be implemented to simulate the dynamic response of a cantilever and calculate the stresses. The model will also be used to predict the deflection amplitude of a cantilever vs. the crack growth length.

## 18. Synthesis and characterization of plasmonic nanoparticle/$TiO_2$ fibre hybrid materials

**Nicole Grobert** Co-Supervisor(s): Barbara Maciejewska

Electrospinning is a well-establish technique using high-voltage to fabricate one-dimensional nano- and microfibres. In conjunction with sol-gel synthesis, it can yield nanostructured ceramics with well-controlled composition and highly modifiable surface properties. $TiO_2$ fibres that synthesized in our lab have proven to be multi-functional materials manifesting great potentials in biomedical applications, catalysis, water treatments, etc.

This project will explore different means to combine plasmonic noble metal nanoparticles with electrospun $TiO_2$ fibres. A variety of material characterization techniques will be involved to study how the metal-semiconductor interaction can affect the structural, optical, electronic, and chemical properties of the hybrid materials. This project will advance fundamental understanding of plasmonic materials and foster their practical applications. The project forms an integral part of the research efforts of the group and is aimed at exploring possible application of these hybrid materials, and where possible in collaboration with industry.

## 19. Fibre reinforced flexible ceramic aerogel for energy, thermal, or structural applications

**Nicole Grobert** Co-Supervisor(s): Barbara Maciejewska

Ceramic aerogels are a diverse class of highly porous solid materials with many appealing properties such as ultralow density, ultra high thermal stability, and excellent chemical resistance. Yet the conventional ceramic aerogels are extremely brittle and fragile, unable to be practically used. Reinforcing the aerogel structure by ceramic fibres is one of the most popular strategies, in which the fibres enhance the flexibility of aerogel, allow tuning the porous structure, and improve the thermal resistance.

This project will exploit using sol-gel synthesis and ambient drying method to fabricate various aerogels, then compositing with the ceramic fibres that have been developed by the Nanomaterials by Design team. The reinforced aerogels will then be characterised, and their properties will be evaluated with view to a series of applications, including gas adsorption, oil/water separation, insulation, etc.

The project forms an integral part of the research efforts of the group and is aimed at exploring possible application of these materials, and where possible in collaboration with industry.

### 20. Synthesis and characterisation of conductive and elastic carbon nanotube aerogels

**Nicole Grobert** Co-Supervisor(s): Barbara Maciejewska

Carbon nanotubes (CNTs) are well-known one-dimensional (1D) nanomaterials possessing extraordinary mechanical, electrical, and thermal properties. The key to open up their extensive applications is assembling CNTs into bulk materials while retaining the desired structures and properties. Our lab has been working on CNT-related materials with current professionals in the synthesising of multi-wall and single-wall CNTs using floating catalyst chemical vapour deposition (FCCVD). This project will start with using FCCVD technique to obtain high quality CNTs, then assembling the CNTs into 3D materials (e.g., bulk aerogels) by means of freeze-drying.

The aim of the project is to understand the effect of different parameters to produce aerogels where the CNT are alignment and entanglement well-controlled. The mechanical properties, electrical conductivity and thermal properties will be evaluated and examined. The potential application of such materials will be in the field of thermal management, catalyst scaffold, battery electrodes, etc. The project forms an integral part of the research efforts of the group and is aimed at exploring possible application of these materials, and where possible in collaboration with industry.

### 21. Tuning the bandgap of $TiO_2$ nanomaterials towards visible-light driven photocatalysts

**Nicole Grobert** Co-Supervisor(s): Barbara Maciejewska

Photocatalytic technologies that harvest solar energy are among the hottest research topics in solving the global energy crisis and environmental issues. Titanium dioxide ($TiO_2$) has been considered as one of the most effective photocatalysts.

Downsizing and nanostructuring of $TiO_2$ lead to a series of superior photocatalysts with strong oxidizing power and exceptional photocatalytic efficiency. Recently, we developed protocols to synthesize various $TiO_2$ nanostructures including nanopowders, nanofibres, and mesoporous microfibres. The photocatalytic efficiency of these materials can be boosted by engineering the bandgap.

The proposed project will involve synthesising $TiO_2$ materials using the sol-gel route. Different dopant atoms will be used to tune the electronic structure of $TiO_2$, therefore manipulating the light absorption especially at visible range. The efficacy of heteroatom doping will be evaluated by photodecomposition of organic dyes. This project will focus on understanding the light-matter interaction towards designing and developing more effective photocatalysts. The project forms an integral part of the research efforts of the group and is aimed at exploring possible application of these hybrid materials, and where possible in collaboration with industry.

### 22. Li alloys for solid state batteries

**Chris Grovenor** Co-Supervisor(s): David Armstrong

Storing the highest energy densities in solid state Li batteries requires the use of metallic Li as the anode, but Li metal is very soft, extraordinarily reactive and difficult to use in practical devices. One idea that is being explored to improve the performance is the formation of high Li content alloys. The simple Li-Mg binary system has been studied extensively and has a wide solid solution range, but does not offer the solution to all the practical difficulties.

This project will make and test novel ternary alloys (with Al, Mg, Sn, Si, Zn) with the aim of controlling the microstructure/mechanical properties to improve the electrochemical performance. Samples will be examined using optical and scanning electron microscopy, EDX and XRD techniques to establish the as-cast microstructure, to measure the mechanical properties, and the more promising materials will be selected for electrochemical testing in coin cells. If the student is interested, it will be possible to learn how to use Thermocalc software to predict the ternary phase diagrams for the selected alloys, and to compare these predictions with the real phase mixtures found in the alloys.

### 23. Exploring ion-exchange methods to make novel multivalent cathodes

**Rob House** Co-Supervisor(s): Peter Bruce

Replacing Li-ion batteries with multivalent ion batteries based on Mg2+ or Ca2+ could lead to significant improvements in cost and capacity, however, there is a lack of suitable cathode materials for these battery systems. One key challenge is that it is not easy to synthesise Mg or Ca-containing layered cathode materials directly. In this project we will investigate exchanging the ions in conventional layered cathodes with Mg or Ca. We will compare the effectiveness of different ion exchange methods, characterise the products and test them in battery cells.

### 24. Disordered rocksalt cathodes for rechargeable Zn batteries

**Rob House** Co-Supervisor(s): Peter Bruce

Single-use disposable alkaline batteries release charge by oxidising Zn at the anode and reducing MnO2 at the cathode in an irreversible chemical reaction. One way to make these batteries rechargeable and significantly reduce waste is to switch to reversible Zn-ion intercalation chemistry. In this project, we will investigate low-cost Mn-based intercalation cathodes for Zn-ion batteries. We will focus on a new class of material known as disordered rocksalts which promise high capacities and reversibility. We will synthesise, characterise and test them in Zn-ion cells.

### 25. Mechanical properties of coatings for nuclear fusion

**Anna Kareer** Co-Supervisor(s): David Armstrong, Angus Wilkinson

For commercially viable nuclear fusion liquid lithium tritium breeder concepts will require a series of coatings to ensure 1) the liquid lithium does not come into contact and react with any underlying metal structure 2) prevent the diffusion of tritium into underlying materials. These coatings must be mechanically viable with both good adhesion to underlying material and adequate mechanical properties in their own right. It will also be important to understand how these degrade during service due to thermal cycling and irradiation damage. In this work a range of transition metal carbides and/or rare earth oxides will be studied using nanoindentation and nanotribology, thermal cycling and SEM based microscopy. The work will be predominantly experimental but analysis will use matlab codes and potentially some finite element modelling

## 26. Low voltage electron ptychography of 2D materials

**Angus Kirkland** Co-Supervisor(s): Chris Allen

Low dimensional materials such as graphene have many potential applications from quantum electronics to highly efficient catalysis. Atomic scale variations in the structure of these materials have profound implications on their macroscopic properties, therefore to fully exploit these materials the correlation between atomic structure and macroscopic properties has to be well understood.

Electron microscopy is a powerful tool for the study of atomic structure of materials, however the high electron energy generally required for atomic resolution imaging tends to cause damage to low dimensional materials, particularly around defect or dopant sites. Imaging at low electron energy should mitigate these damage problems but due significantly poorer spatial resolution atomic structure determination is not possible.

Electron ptychography is a cutting-edge imaging technique which enables image resolutions beyond the optical limits of standard imaging modes. It has also been shown to be very dose efficient with high signal to noise images reconstructed using relatively few incident electrons.

In this project we will use low voltage electron ptychographic imaging to determine the intrinsic structure of edges, defects and dopants in graphene. The project will involve experimental data acquisition of world leading electron microscopes, computational reconstruction of images using existing in-house codes and image simulation for experimental design and result validation.

The candidate would have an interest in structural characterisation and should have good computational skills. They will also be required to travel to Harwell for meetings and for the experimental work.

## 27. Artificial Intelligence for multi-modal X-ray Imaging of metal solidification

**Enzo Liotti** Co-Supervisor(s): Andrew Zisserman (Engineering)

X-ray imaging techniques using synchrotron sources have emerged as a powerful tool to study the dynamics of crystal growth, however, the vast and complex data sets generated during multi-modal time-resolved experiments present profound technical and practical problems for quantification. Applying artificial intelligence to X-ray imaging, including by our group (Liotti et al., Science Advances (2018)), has so far mainly focused on speeding up cumbersome human operations on uni-modal tomographic data, such as volume reconstruction and segmentation, and radiograph post-acquisition analysis. Little work has been carried out on multi-modal deep learning, which therefore remains a difficult challenge as well as an enormous opportunity.

The project will focus on the development of algorithms for real-time analysis. Self-supervised vision transformers will be trained for a set of core tasks, such as identification of different solid phases, both in aluminium alloys and steel, and measuring their nucleation and growth rates. These models will then be further trained for more complex tasks to shed light on the interdependency of all the phenomena taking place during metal processing and understand the relationship between the dynamical evolution of microstructure during solidification and the subsequent solid-state transformations.

## 28. Characterization of aluminium secondary phase nucleation using thin film deposition and high-resolution electron microscopy

**Enzo Liotti** Co-Supervisor(s): Shikang Feng, Andrew Watt

Controlling the nucleation and growth of secondary phases in aluminium alloys is a primary challenge in the development of greener materials. The heterogeneous nucleation science for solid phases forming during solidification has been developed only for cubic solid solutions using well-known, empirically discovered nucleants such as aluminium nucleation on $TiB_2$. Secondary phases are often ordered intermetallic compounds (IMCs) with complex, low symmetry crystal structures resulting in a multitude of dissimilar planes and directions characterised by different packing densities and surface energies. This anisotropy affects the growth behaviour, but it is not known how it may affect, or might be exploited for, IMC nucleation.

The project will experimentally investigate the nucleation behaviour of a selected group of candidate inoculants to characterise the nucleant/IMC interface chemistry and crystallography. Samples with a large contact area between the nucleant material and the alloy forming the IMC under investigation will be fabricated, for each nucleant/IMC pair, via thin film deposition and Field Assisted Sintering Technology (FAST) and analysed by high-resolution SEM using EBSD and EDS. The data will be used to estimate the efficacy of the nucleants, study the ORs and investigate other phenomena such as the effect of minor elemental additions on nucleation potency and the efficacy of the nucleant due to alteration of the chemistry at the interface between nucleant and nuclei.

### 29. High-resolution characterization of metal powders for Additive Manufacturing of space materials

**Sergio Lozano-Perez** Co-Supervisor(s): Neil Young

This project is in collaboration with the European Space Agency (ESA), which has an interest on using additive manufacturing for producing space hardware. One topic of particular interest is the control of the raw material. Metallic powders can be produced in different grades of quality and only the highest performing powder is selected for producing space parts. This Part II project aims to improve the understanding of powder characteristics by utilising methods such as Focused Ion Beam (FIB), high resolution Electron Microscopy (SEM) and related analytical methods (EDX).

### 30. Analysis of in situ high resolution synchrotron tomography of graphite fracture

**James Marrow**

Graphite is used as a neutron moderator in high temperature nuclear reactors. Its fracture toughness depends on the relative strengths of the filler particles and binder matrix, which may age differently. Multi-dimensional observation and analysis of crack propagation can be used to study fracture resistance (http://dx.doi.org/10.1016/j.carbon.2020.09.072). A recent tomography experiment at the PSICHE beamloine of the SOLEIL light source (20190926) has obtained images for crack propagation in nuclear graphite at unprecedented spatial and temporal resolution and with large field of view.

This project asks the question “Can the local fracture resistance of matrix and filler within the heterogeneous and porous graphite structure be quantified?” This is a data analysis project, so no new experiments will be done. You will need to devise an efficient analysis method to extract and correlate the crack’s 3D strain fields with their local microstructure using a large dataset. You will also apply state-of-art visualisation, machine-learning based segmentation and digital correlation analysis software (Avizo). The output will lead to improved modelling of the strength of nuclear graphites.

## 31. Synchrotron X-ray imaging and diffraction analysis of tensile deformation of a ceramic composite

**James Marrow**

3D needle-punched carbon fibre felts or non-woven cloths are used as the reinforcement in C/C and C/C-SiC composites. To understand how their damage tolerance is affected by process variables (e.g. thermal stresses) and composite architecture, it is important to observe how damage initiates and propagates (https://doi.org/10.1016/J.COMPSTRUCT.2018.11.041).

This project asks the question "How does the propagation of cracks in the matrix and fibre bundles interact with the process-induced residual stresses?". This is information needed to validate image-based models of composite behaviour (e.g. https://doi.org/10.1111/ffe.12537). A unique experiment has been performed at the Diamond Light Source (EE17360) to examine the tensile deformation of a 3D needle-stitched C/C-SiC ceramic composite. High resolution computed tomography was combined with diffraction observations to examine the evolution of cracking and stress partitioning between the composite constituents. You will need to combine 3D strain mapping by digital image correlation of tomographs with 2D mapping of the crystal strains by analysis of monochromatic Bragg diffraction data (e.g. https://doi.org/10.1016/j.carbon.2020.03.020) to correlate the evolution of stress, strain and damage in a large and complex dataset. This is a data analysis project, so no new experiments will be done. You will be using state-of-art visualisation (Avizo) and diffraction analysis (DAWN) tools, with opportunity to develop novel data visualisation and numerical analyses.

## 32. In situ Studies of the Deformation of Highly Porous 3D CNT tube (CNTT) Networks

**James Marrow** Co-Supervisor(s): Nicola Pugno (Trente University)

Highly porous 3D CNT tube (CNTT) networks have interesting mechanical and electrical properties with potential applications in technologies that include stretchable conductors, gas sensing, cell-scaffold materials, and cathode materials for batteries. A novel material has been developed (at Keil University) with mechanical properties and electrical properties that are enhanced by CNT networks, self-entangled around a highly porous 3D zinc oxide ceramic 'tetrapod' foam (https://doi.org/10.1038/s41467-017-02372-9). It has an open structure with a high porosity, which is beneficial for several applications due to high surface accessibility. The ceramic can be dissolved to leave the CNTT network.

This project asks the question "How does the network deform, and is it uniform or heterogeneous?" This question can only be answered by in situ observations, obtained within the three-dimensional material. Following on from previous Part II studies of the ZnO template, (https://doi.org/10.1016/j.scriptamat.2022.115153), you will design experiments to study the cyclic deformation and failure of CNTT materials, using in situ, high resolution computed X-ray tomography. Deformation and fracture will be quantified using digital volume correlation, as a function of the applied strain. The project will involve mechanical testing, computed tomography, data visualisation and numerical analysis (Matlab), with opportunities to apply finite element simulation.

## 33. Fracture Resistance of thermally oxidised graphite

**James Marrow**

There is a need to measure the fracture toughness and resistance to stress concentrating notches in fine grained nuclear graphites that are the proposed structural materials for next generation high temperature and molten salt nuclear fission reactors. These graphites will be exposed to irradiation, oxidation and corrosion and cannot be replaced during the reactor life. Materials test reactors are used to provide accelerated irradiation tests to qualify and select materials, but there are severe restrictions imposed on the sample dimensions. Hence there is to test small specimens to measure properties.

A novel method has been developed to evaluate the stress intensity factor by measurements of displacement field around the crack tip (http://dx.doi.org/10.1007/s11340-017-0275-1, https://doi.org/10.1016/j.jnucmat.2022.153642), and a recent Part II showed this could be applied to graphite (https://doi.org/10.1520/STP163920210051)

This project asks the question “What is the effect of oxidation of the graphite microstructure on the fracture toughness?”. This experimental study will use optical DIC and DVC of tomographs to measure, in situ, the displacement fields of a centre-hole notched compression specimens during crack propagation tests. The effects of oxidation on the elastic properties and toughness will be investigated - effects of thermal oxidation on the graphite microstructure have already been examined, using computed X-ray tomography. The elastic properties and fracture toughness will be evaluated from these data. The analysis will require some use of finite element modelling methods, and also post-processing of data using tools written in Matlab.

### 34. In situ study of the compressive failure of densified wood

**James Marrow**

Natural wood is a low-cost and abundant material, but its mechanical performance is unsatisfactory for many advanced engineering structures and applications. Existing pre-treatments (heat/steam etc) can enhance its mechanical properties, but result in incomplete densification and lack dimensional stability, particularly in response to humid environments. Novel processes [https://doi.org/10.1038/nature25476, https://doi.org/10.1016/j.matt.2021.09.020] can now transform natural wood directly into a high-performance structural material with a more than tenfold increase in strength, toughness and ballistic resistance and with greater dimensional stability. The processed wood has a specific strength higher than that of most structural metals and alloys, making it a low-cost, high-performance, lightweight alternative. Proposed applications include a honeycomb core material for battery containment in vehicles.

In this project, which is in collaboration with Dr Ning Jiang (Shandong University of Technology, China), you will study the compressive failure of natural and densified pine using in situ high resolution X-ray tomography, analysed by digital volume correlation, to observe the microstructure and mechanisms of damage evolution. The development of damage in sections of honeycomb densified wood will also be examined, to investigate anisotropy and heterogeneity and the materials response to stress concentrations. The project will involve mechanical testing, computed tomography and data visualisation. It may involve numerical analysis (Matlab), with opportunities to apply finite element simulation with inverse modelling to extract material properties.

### 35. APT investigation of ceramic coatings to prevent tritium permeation in nuclear fusion reactors

**Michael Moody** Co-Supervisor(s): Paul Bagot, Hazel Gardner (UKAEA)

Future reactor designs such as DEMO and STEP will breed large quantities of tritium fuel and maintaining tritium inventory is essential to safe and efficient plant operation. Thin (micron-scale) multilayer coatings are one way to control tritium diffusion and are an active area of materials development. Erbium oxide barriers provide significant trinity permeation reduction, however, experimental measurements quantifying this protection in the literature can vary and are often orders of magnitude lower than theoretical predictions, making it difficult to accurately predict and validate coating performance. A key reason for this is a limited understanding of hydrogen isotope trapping and transport behaviour within ceramic coatings, which could be addressed through quantification and spatial mapping of hydrogen isotopes within the coating and at the coating-substrate interface. The high spatial resolution and chemical sensitivity of atom probe tomography (APT) has previously enabled quantification and mapping of hydrogen at microstructural features in steels.

This project will apply the APT technique to erbium oxide coatings to address the knowledge gap around hydrogen isotope transport and trapping in ceramic oxides, with the ultimate aim of improving coating lifetime predictions.

## 36. Investigating the atomic-scale irradiation damage in an Inconel 617 superalloy

**Michael Moody** Co-Supervisor(s): Paul Bagot, Christina Hofer

Inconel 617 nickel-based alloy is a candidate material for components with a variety of applications in Gen IV fission reactors. However, significant research is still required to characterise this alloy's microstructural response, and hence degradation in mechanical properties, when subject to a combination of irradiation and elevated temperatures.

This project, in collaboration with the Australian Nuclear Science and Technology Organisation (ANSTO), will implement atom probe tomography (APT) for atomic-scale characterisation of Inconel 617 microstructure evolution when systematically subjected to a combination of heat treatments and ion irradiation.

## 37. Transport and thermodynamic properties of Zn-ion electrolytes

**Mauro Pasta**

Knowledge of electrolyte transport and thermodynamic properties in rechargeable batteries is vital for their continued development and success. Our group has recently introduced a new method to fully characterize electrolyte systems. [Fawdon et. al. 2021] By measuring the electrolyte concentration gradient over time via operando Raman microspectroscopy, in tandem with potentiostatic electrochemical impedance spectroscopy, the Fickian "apparent" diffusion coefficient, transference number, thermodynamic factor, ionic conductivity and resistance of charge-transfer can be quantified within a single experimental setup.

In this project, the student will use operando Raman microspectroscopy to investigate the transport and thermodynamic properties of Zn-ion electrolytes and their correlation to Zn-dendrite nucleation and propagation in Zn and Zn-alloy anodes.

## 38. Zn-alloy anodes

**Mauro Pasta**

Zinc-air batteries are particularly well suited for stationary storage in weak- and off-grid applications: they afford large theoretical energy density (1353 Whkg-1), inherent safety (aqueous electrolyte), potential for extremely low costs (<25 $ kWh-1), and good recyclability [Shang et. al. 2022]. ZABs were first commercialized in 2012 but still suffer today from limited energy density and cost >100 $ kWh-1 [Zhang et. al. 2019]. One of the key scientific challenges that must be addressed to release the potential of ZABs is the growth of dendrites on the Zn metal anode during recharge which results in poor cyclability and side reactions (e.g., hydrogen evolution), impacting both cyclability and coulombic efficiency.

In this project the student will explore the effect of alloying Zn on the kinetics of both the H2 evolution reaction and Zn plating and stripping.

## 39. Compact nutrient sensors for water quality monitoring

**Jason Smith**

Nutrients such as nitrates and phosphates are major sources of pollution in waterways, causing algal blooms and threats to health, and there is a global need for improved sensors to monitor their levels. In this project you will design, fabricate and test new compact optical sensors based on microcavity technology developed within the group. The project will be carried out in communication with a new commercial enterprise with a view to their industrial application.

## 40. Modelling a quantum computer based on colour centres in diamond

**Jason Smith**

Colour centres in wide band gap materials such as diamond have strong potential for use as physical qubits in large scale quantum computers, but detailed models of how quantum information will be processed in such systems have yet to be developed. In this project you will use a flexible computer modelling platform, the Quantum Exact Simulation Toolkit (QuEST), to simulate elements of a diamond quantum computer based on distributed entanglement between colour centres across a network.

The project will involve developing models of ‘toy systems’ based on the unique connectivity and established gate times and error rates. The goal of the project is to develop our understanding of how best to implement these quantum computers in practice.

### 41. Analysis of irradiation damage in atomic resolution STEM images of high temperature superconductors

**Susie Speller** Co-Supervisor(s): Peter Nellist

High temperature superconductors are an essential enabling technology for compact nuclear fusion power plants. In operation, the highly sensitive superconducting material will be exposed to a high flux of energetic neutrons released by the fusion reaction that create structural defects that degrade superconductivity. However, very little is known about the nature of the defects that are created, and whether other projectiles (such as light ions that are easier to work with) can replicate the same kind of damage.

This project involves developing image analysis and applying simulation techniques to analyse existing high quality atomic resolution scanning transmission electron micrographs on pristine, ion irradiated and neutron irradiated high temperature superconductors, with the aim of quantifying irradiation induced disorder and structural changes.

### 42. Superconducting thin films for quantum devices

**Susie Speller** Co-Supervisor(s): Clara Barker

Qubits and resonators are the building blocks for quantum computers but material challenges significantly limit their potential, with current materials used for convenience rather than by design. This project will carry out fundamental investigations of promising materials for resonators in quantum devices. Thin films will be made using magnetron sputtering, and their material properties tested thorough microstructural characterisation and measurement of superconducting properties. These films will be tested for suitability as quantum resonators, as part of a larger project. The main goal of this project will be to study more novel superconducting materials for use in quantum devices, such as Mo:Re and MoN.

## 43. Persistent joints in high temperature superconductors

**Susie Speller** Co-Supervisor(s): Chris Grovenor

The large magnets required for applications in medical MRI and large physics experiments like the LHC at CERN are all based on superconductors, and can contain numerous joints that are often the (very expensive) points of failure. Reliable processing strategies are needed to prepare joints between shorter lengths of wire with resistances lower than $10^{-13}\,\Omega$.

This project will work with our partners in Oxford Instruments on making and testing joints between Bi-2212 superconducting wires – how to improve reliability and performance, and understanding what goes wrong. The project will involve improving joint making processes that are based on a melting and peritectic reaction process, using XRD and analytical SEM to analyse the phase purity and microstructure of the joints, and measuring the persistent performance of small coils by measuring the decay of induced currents.

## 44. Improving the reliability of solid state battery electrolytes and other ceramics by surface residual stress

**Richard Todd**

Solid state lithium batteries offer improved energy density and safety but suffer from short circuiting or fracture owing to the growth of lithium dendrites into the solid electrolyte. This should be suppressed by incorporating compressive surface stresses in the electrolyte and preliminary results have been encouraging. The project will develop this idea further using laminated electrolytes and/or other methods of producing residual stress. The project will involve ceramic processing and the characterisation of microstructure, mechanical properties and electrochemical performance.

## 45. Metal Nanowire Based Devices for Ambulatory Blood Pressure Monitoring

**Andrew Watt** Co-Supervisor(s): Helen Townley (Women's Reproductive Health)

Recently we demonstrated that we could build a nanowire-based pressure sensor with sufficient sensitivity and mechanical properties to measure changes in venal flow. We wish to build upon this exciting initial result and show that it is possible to make a passive measurement of blood pressure.

The project will involve nanowire synthesis and device fabrication alongside ex vivo testing and a variety of materials characterisation techniques.

### 46. Quantum Dot Photovoltaics

**Andrew Watt** Co-Supervisor(s): Sebastian Bonilla

The efficiency of solution processed lead chalcogenide colloidal quantum dot (CQD) solar cells has increased from less than 1 to over 15% in the last 12 years. They have proven to be air-stable and do not require high temperature processing, which are major drawbacks for competing thin film, organic, perovskite and dye sensitized technologies. A project is offered with one of the following focuses 1. CQD Syntheisis 2. CQD Device Characterisation 3.CQD TEM. All projects will involve the fabrication of devices.

### 47. Advanced Metallisation Technology for Next-Generation Photovoltaics

**Andrew Watt** Co-Supervisor(s): Sebastian Bonilla

Solar photovoltaic cells use metal contacts made primarily of screen-printed silver, and in some cell designs the metallisation also requires a transparent conducting film of indium tin oxide. The use of these materials is currently limiting further reductions in cell manufacturing cost, with the metals used contributing as much as one quarter of the cost of the cell. The ongoing trend to reduce the price of solar panels requires the shift towards a metallisation schemes that minimise the use of such expensive or nonabundant materials.

This project aims to explore novel contact and metallisation technologies that can address this critical hurdle for the future of solar electricity generation, using solvo-dynamic printed nanowire high aspect ratio contact electrodes. Silver-free metal to semiconductor contacts will be explored in collaboration with our international partners, and new technologies will be proposed to achieve low-cost manufacturing of efficient metallisation for single and multijunction solar cells. Analytical and electrical characterisation techniques will be used to assess the performance of the metallisation, including advanced nano scale mass-spectroscopy and electrical current transport. The understanding and development from this project will result in improved manufacturing of commercial solar panels, which in turn will help mitigate the devastating consequences of climate change.

## 48. Direct-formation of suspended 2D material membranes

**Robert Weatherup**

X-ray Photoelectron Spectroscopy is one of the most powerful techniques for obtaining surface-sensitive chemical information, by detecting photoelectrons that escape from within a few nm of a surface. However it is typically restricted to solid surfaces under vacuum conditions, limiting its potential applications.
This project will involve the development of ultra-thin and impermeable 2D material membranes (Graphene/Tungsten Disulphide) for encapsulating liquids, so that they can be measured using XPS. This will include learning to produce 2D materials by chemical vapour deposition (CVD), and then optimising growth on metal layers suspend on perforated supports. The metal can then be etched away to leave the suspended 2D material membrane. These will then be characterised optically and with scanning electron microscopy before testing in a vacuum chamber to confirm they are leak-tight. They can then be used for observing liquid-phase catalytic reactions or the accumulation of ions on the surface of the 2D material under electrochemical bias using lab-based XPS systems in the department.

## 49. Investigating the role of additives on lithium-ion battery lifetime

**Robert Weatherup** Co-Supervisor(s): Erik Bjorklund

Lithium-ion batteries are already widely deployed in portable electronics and increasingly in electric vehicles. To maximize the energy that can be stored it is desirable increase the voltage to which they can be charged, however the $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$(NMC) materials commonly used as cathodes are not very stable at high potentials. In order to prolong battery lifetime approaches are needed to stabilise NMC surfaces at high potentials.
In this project we will study different electrolyte additives to suppress unwanted side reactions causing battery degradation. Electrochemical measurements will be performed to evaluate how effective these different additives are in stabilizing the NMC surface, and this will be followed by characterization with various techniques determine how the additives interact with the NMC electrode. This is likely to include x-ray photoelectron spectroscopy (XPS), x-ray absorption spectroscopy (XAS), Differential electrochemical mass spectrometry (DEMS) and electrochemical impedance spectroscopy, but there will be scope to explore other methods as the project progresses.

## 50. Revealing edge sites in graphite electrodes for Li-ion batteries

**Robert Weatherup** Co-Supervisor(s): Pravin Didwal

Graphite is widely used as the anode in lithium-ion batteries, where lithium can be repeatedly inserted and removed from between its layers as the battery is charged and discharged. Alongside this reversible reaction, irreversible electrolyte decomposition can occur at the graphite surface. The extent of these irreversible reactions are thought to be significantly increased by the presence of graphite edges. Understanding the performance of different graphite electrodes thus requires an understanding on the proportion their surface associated with graphite edges compared to the less reactive basal plane.

This project aims to develop an elegant approach to determine this based on the enhanced catalytic activity of these edges. Electrochemical reactions will be used to study well-defined graphene layers to determine the relationship between reaction rate and edge density. This will then be extended to a variety of commercially available graphite electrodes. This will involve correlating electrochemical data with experimental characterisation of microstructure (Electron and optical microscopies) and surface area (BET method). Ultimately the aim is to correlate edge density with the irreversible capacity lost in real Li-ion batteries.

## 51. Size-selected multi-component alloy nanoparticles for electrochemical hydrogen production

**Robert Weatherup** Co-Supervisor(s): Leanne Jones

The production of hydrogen by electrochemical splitting of water offers a zero-carbon method for converting renewable energy to a fuel which can be stored for when it is needed and used to replace fossil fuels in many industrial processes. To produce hydrogen efficiently, electrocatalysts are needed that reduce the overpotential and avoid large amounts of energy being wasted. Alloy nanoparticle catalysts are particularly promising as they offer high surface areas, and their catalytic performance can be tuned by their size and composition. However, rational improvement of performance requires the deposition of a large number of nanoparticles of well-defined size and composition.

This project will use a newly installed deposition source, that forms nanoparticles of controlled size by expanding a metal vapour through a nozzle, and then mass filters these to select only particles of a desired size. The formation of high entropy alloy particles (containing >5 elements in roughly equal proportions) will be studied and then their sizes and variation in composition characterised using electron microscopy, and X-ray photoelectron spectroscopy. The performance of optimised catalysts will then be investigated for electrochemical water splitting.

## 52. Developing surrogate modelling strategies for crystal plasticity parameter determination

**Angus Wilkinson**

Establishing materials parameters for crystal plasticity simulations is often conducted by user iteration and judgement of an acceptable fit to experiment. This is unsatisfactory as the process is labour intensive and the results subjective. This project will explore machine learning approaches to generate surrogate models, trained on data from full crystal plasticity simulations. The surrogate models will be approximate but fast and constructed to solve the inverse problem giving best estimates of materials parameters directly from observed experimental data (which cannot be directly done from the full crystal plasticity simulation).

The material property parameters we seek include: elastic constants, critical resolved shear stress, activation energies and volumes (or strain rate sensitivities), while the experimental observables include bulk stress-strain-time response, along with lattice strain evolution from in situ XRD, or spatially resolved strains from DIC. We will start simple and build up the complexity and number of parameters and observables as the project progresses, using experimental datasets already measured by the group.

## 53. Effects of hydrogen on mechanical behaviour of steels

**Angus Wilkinson** Co-Supervisor(s): David Armstrong, Phani Karamched

Zero carbon energy systems are needed urgently. Gas is used for heating in 85% of households in the UK and this could be replaced by hydrogen supplied through the existing national transmission system (NTS).

Assessing the potential effects of hydrogen on pipeline steels is a necessary part of the safety case. Ferritic-pearlitic steels are used in the main high-pressure pipelines and potential detrimental effects include hydrogen embrittlement and accelerated fatigue crack growth.

Using a new in-situ electrochemical nanoindentation cell this project will compare the mechanical behaviour of such steels with and without hydrogen charging. Combinations of ex-situ and in-situ mechanical testing, with digital image correlation (optical and SEM imaging), will be used along with HR-EBSD, and AFM characterisation.

### 54. Micromechanical Measurements of Manufactured Moon Metal

**Angus Wilkinson** Co-Supervisor(s): David Armstrong, Martina Meisnar (ESA)

As human spaceflight returns its focus to the moon, creating safe longer-term habitats will be necessary. In situ resource utilisation (ISRU) would seem a requirement and one possible route is to use local lunar regolith material (soil) as the starting material. Advances in-space processing have demonstrated that lunar regolith can be reduced to provide oxygen (needed for fuel) which leaves a mixed metal waste stream, containing a range of structural metals including iron, titanium, magnesium and aluminium, but also calcium and silicon. There is potential for using this metal for lunar based manufacturing, but much characterisation on the powder's properties is needed.

The project consists of characterising simulated reduced lunar regolith derived metal with the aim to understand its properties for use as additively manufacturing a moon base. Correlative nanoindentation and surface microscopy methods will be used to explore chemistry-structure-properties relationships at the microscale with the aim of developing better micromechanical understanding of these unusual materials. This work will be carried out on both base powder and sintered materials. The project will involve close collaboration with engineers at the European Space Agency.

## 55. Novel, low-cost approaches to ‘STEM-in-SEM’ electron microscopy

**Neil Young** Co-Supervisor(s): Ian Griffiths

Lab-based 3D printing techniques are currently being developed in support of electron microscopy characterisation methods. This cheap and high-throughput fabrication technique is proving to be a disruptive innovation; dramatically increasing the possibilities for electron microscopy ancillaries and consumables and enabling rapid deployment of novel experiments.

In this project you will work on the design, fabrication and development of a transmission imaging attachment for a conventional scanning electron microscope (STEM-in-SEM). This will involve the fabrication of 3D-printed test structures and use of the mechanical workshops to produce a hybrid ‘metal-3D printed’ working prototype. This will be tested in a range of SEM’s available in the David Cockayne Centre for Electron Microscopy. 3D printing will also be used to develop novel specimen holders for analysis of bulk and nanomaterial specimens. The project will suit a student wishing to gain hands-on experience with electron microscopes and the mechanical workshop.

## 56. Understanding ion damage in TEM specimen preparation, comparing Ar, Ga and Xe ions.

**Neil Young Co-Supervisor(s): Ian Griffiths, Gareth Hughes**

Artefact-free specimen preparation is essential in performing advanced materials characterising via electron microscopy. In this project you will use an Ar-ion milling system to explore the interaction of Ar ions with a range of EM specimen geometries. The role of Ar-ions in polishing semiconductor specimens and removing artefacts will be explored via a systematic approach. As the project progresses FIB techniques will be introduced allowing the damage rate from Ar, Ga and Xe ion beams to be compared.

The project would suit a student with a deep interest in materials characterisation techniques and instrumentation. An organised and careful approach to practical work would be required. The student would gain hands-on skills across a range of electron microscopy techniques and practical specimen preparation.

## 57. Structural studies of supported metal nanoparticles and catalyst materials

**Neil Young**

The atomic structure of metal nanoparticles is of direct importance to numerous nanotechnology applications. Combining direct visualisation of nanoparticle structure via high-resolution TEM, with in-situ and ex-situ heating allows for nano-structural phase diagrams to be established. These give a thermodynamically robust account of nanoparticle atomic structure as a function of size and temperature. You will continue the work of previous PtII students and focus on platinum nanoparticles and their interaction with various support materials, including commercial catalyst materials. The student would gain hands-on skills across a range of electron microscopy techniques and practical specimen preparation.

## 58. DFT modelling of battery materials

**Rebecca Nicholls** Co-Supervisor(s): Saiful Islam

Next generation lithium ion batteries are limited by the cathode material and an incomplete understanding of how the material behaves during operation and degradation. Spectroscopic signals generated by both electron and X-ray beams can be used to probe charged or degraded materials. This project will use first-principles calculations to simulate spectra from a variety of pristine and charged/defective materials to explore the possibility of using spectroscopy as a way of understanding the operation and degradation of battery materials for potential electric vehicle applications.

## 59. Modelling adsorption and assembly of nucleobases on gold surfaces

**Chris Patrick** Co-Supervisor(s): Martin Castell

Nucleobase molecules like adenine, guanine and cytosine are the basic building blocks of DNA and RNA. One way of studying how the molecules interact with each other is to place them onto an inert surface like Au and image them using scanning tunnelling microscopy (STM). Complementary to the experiments, first-principles electronic structure calculations based on density-functional theory can be used to predict the structures likely to be formed, and also to provide a way of interpreting the experimental images. However, modelling these systems is made more complicated by the relatively weak bonding (physisorption) that they undergo, which is not particularly well described by standard approximations to DFT.

The first part of this modelling project will therefore involve critically assessing the performance of established and recently developed exchange-correlation functionals in describing these molecules, with the opportunity to perform high-accuracy "post-DFT" calculations in order to generate benchmark data. The second part of the project will focus on using the established calculation protocol to parameterize a larger-scale model of the network formed by the multitude of molecules interacting on the surface. As such, this challenging project will require the student both to carry out careful and precise numerical calculations and also to devise a physical model to understand this complicated system.

## 60. Structural and electronic properties of metallic monolayers on oxide surfaces

**Chris Patrick** Co-Supervisor(s): Martin Castell

The properties of materials can dramatically change if they are forced to adopt low-dimensional structures. Such structures tend only to be stable in the presence of a second material, as is the case with a monolayer of atoms formed on top of a substrate. In this case, it is possible that the structure of the monolayer, and its associated properties, will be determined by the precise nature of the substrate. This modelling project focuses on Au atoms adsorbed on the perovskite-type oxide SrTiO_3, and will use first-principles density-functional theory calculations to build different potential models of the interface, with a view to finding the most stable structure. The electronic properties will be calculated and compared to the bulk materials. The calculated structures will be used to simulate scanning tunnelling microscopy images to be compared to experimentally-measured data.

This project would suit a student interested in learning how computational materials modelling can be applied to problems in surface science. As well as computational skills and an interest in electronic structure, strong crystallography skills are also a prerequisite for this project.

## 61. Understanding magnetostriction in Laves phase rare earth compounds

**Chris Patrick** Co-Supervisor(s): Jonathan Yates

Magnetostriction is the property where applying a magnetic field to a material causes it to undergo strain. Since this phenomenon couples electromagnetic and mechanical energy, magnetostrictive materials have applications in sensors and actuators. "Terfenol-D" has the highest magnetostriction of all known materials and is an alloy of iron with the rare earth metals terbium and dysprosium, with the formula Tb_{1-x}Dy_xFe_2. Terfenol-D crystallizes in the cubic Laves phase, and its extraordinary magnetostrictive properties must originate from this well-known crystal structure. However, despite Terfenol-D having been discovered decades ago, the exact mechanism which generates this huge magnetostriction remains unknown.
In this modelling project we will combine state-of-the-art techniques based on density-functional theory with simpler equations from electromagnetism to attempt to obtain new insight into the magnetostriction process.

The project will involve studying the theory, setting up and running calculations, and then using the results to fit analytical models. As such, it would suit a student with a strong interest in computational modelling and theoretical development, comfortable with the electromagnetism studied at prelims and wanting to use their mathematical training to tackle a difficult problem.

### 62. Investigating the coupling of electronic properties with atomistic structure with different exchange-correlation functionals

**Chris Patrick** Co-supervisor (s): Jonathan Yates

The starting point for electronic structure calculations is usually that the nuclei are objects fixed in space, and the computational effort is concentrated on understanding the behaviour of electrons. However, a material's electronic properties are affected by the position and motion of the nuclei, most notably in all phenomena involving the "electron-phonon interaction" like superconductivity and indirect optical absorption. Electron-phonon properties have been successfully calculated within density-functional theory for many years, but the field remains under active development, not least due to the high computational cost involved in some of the calculations.

In this modelling project we will take recently developed methods to calculate electron-phonon effects on bandstructure and optical properties and perform a quantitative investigation on the role played by the exchange-correlation functional, in particular comparing generalized-gradient approximations (GGAs) with the more advanced meta-GGA approach. These methods involve a certain degree of statistical analysis and population sampling, and may require the student to generate and manage rather large datasets. As a result, this project requires the student to be interested both in electronic structure theory and also computational aspects, e.g. the use of Python for scripting and data analysis.

## 63. Modelling the activity of Cu, Zn and CuZn catalysts for methanol generation

**Robert Weatherup** Co-Supervisor(s): Rebecca Nicholls, Jack Swallow

Methanol is promising as a low-carbon fuel and liquid hydrogen carrier, where synthesis by hydrogenation of $CO_2$ offers a means of utilizing captured $CO_2$ that, when combined with $H_2$ produced by electrochemical water splitting, yields zero or even negative carbon emissions. Cu/ZnO-based catalysts are extensively used for industrial methanol synthesis, with activation of $CO_2$ by Cu well-established, however the exact role of ZnO in promoting methanol production over other possible products remains hotly debated. Several possibilities have been suggested including ZnO acting as a hydrogen reservoir, an oxygen reservoir, or leading to forming a bifunctional alloy.

This project aims to use Density Functional Theory (DFT) to investigate two key reactions which are integral to methanol synthesis from $CO_2$: $CO_2$ activation and $H_2$ dissociation. Slabs of Cu, Zn, CuZn will be created to determine the $CO_2$ absorption and activation energy, and $H_2$ dissociation energy on different sites. This will provide insights into the role of ZnO including if there is any synergistic enhancement to Cu sites.

## 64. Computational Study of Frenkel defects for quantum technologies

**Jonathan Yates** Co-Supervisor(s): Jason Smith

Point defects in crystalline semiconductors and insulators are leading candidates for solid-state qubits in quantum technologies. It is important to develop techniques which give control over the spatial distribution of such defects. Direct laser writing with single ultrafast pulses has recently been shown as a promising way to excite isolated Frenkel defects (bound vacancy-interstitial pairs) in diamond at desired locations, such that subsequent annealing can produce high-quality vacancy centres.

The objective of this project is to use Materials Modelling techniques to study the interactions of such Frenkel defects for a range of Group IV elements, to understand and inform ongoing experiments. This project will involve large-scale DFT calculations using local and national supercomputing resources. There will be close interaction with experimental work taking place in the Materials and Engineering departments.

## 65. Machine Learning in Materials Modelling

**Jonathan Yates** Co-Supervisor(s): Volker Deringer (Chemistry)

Modern computational methods such as DFT are well suited to the study of perfectly crystalline materials. However, the study of amorphous materials – critical to a wide range of technologies – is challenging. Machine learning offers a route to simulating large systems at low cost with DFT accuracy. Deringer has worked extensively on machined-learned potentials for structural studies. What is needed now is the ability to machine-learn experimental observables such as NMR or EEL spectra. This project will address this missing step – crucial for machine-learning techniques to truly inform experimental work. This project will involve a degree of python usage and development. Students should either have such skills, or be willing to develop them in the early stages of the project.

## 66. Modelling New Materials for Rechargeable Batteries

**Jonathan Yates** Co-Supervisor(s): Saiful Islam

Materials performance lies at the heart of the development of green energy technologies such as lithium-ion batteries, and computational methods now play a vital role in modelling and predicting the properties of complex materials. For the rechargeable lithium battery, the positive electrode is one of the major challenges for new electronics and electric vehicles. In addition, there is a growing interest in sodium batteries as the high sodium abundance makes them attractive candidates for low cost grid-storage.

We propose a Part II project using advanced computer modelling techniques to investigate new oxide and oxyfluoride cathode materials for lithium- and sodium-ion batteries. The DFT-based simulations will examine structural, electronic and ion diffusion properties. Overall, we will examine factors that may enhance the energy density and charge/discharge rate of novel battery materials.

**Recent Paper on modelling cathodes**

Sharpe R, et al., ‘Redox Chemistry and the Role of Trapped Molecular O2 in Li-Rich Disordered Rocksalt Oxyfluoride Cathodes’, *J. Am. Chem. Soc.* **142**, 21799–21809 (2020)

**Review on modelling cathodes**

Islam M S and Fisher C A J, ‘Lithium and sodium battery cathode materials: computational insights into voltage, diffusion and nanostructural properties’, *Chem. Soc. Rev.*, **43**, 185-204 (2014) .