# PhD Studentships in the Department of Materials Science University of Cambridge

This document lists project studentships which are fully funded and usually available immediately, if not then usually they are available from the start of the next academic year. The majority are available to 'home rate fee' paying students only.

For other information, please contact:
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Please include a CV and state your project(s) of interest.

# PhD Studentships



## Fully-funded PhD studentships

### PhD Studentship: Multi-Dimensional Electron Diffraction: New Technology and Data Analytics for Improved Pharmaceutical Understanding and Performance

Sponsor: supported by GSK through an EPSRC Industrial CASE award
Supervisor: Prof Paul Midgley
Start date: 1 October 2021, duration 4 years
Closing Date: 31 January 2021

Determining the atomic structure (and hence properties) of small molecule compounds is at the core of analytical and materials science activities across the pharmaceutical industry. Single crystal X-ray diffraction is regarded as the ‘gold standard’ structure determination technique but generally requires (relatively large) custom-grown crystals, which can be a significant bottleneck and may not be representative of the material that results from manufacturing, processing and subsequent formulation. The emerging technique of low-dose multi-dimensional electron diffraction, with its ability to study nanoscale-sized crystals, has the potential to be a major step-change for structure determination for the pharmaceutical industry.

In this project we will we develop two forms of multi-dimensional electron diffraction. Firstly, 3D electron diffraction (3D-ED), or ‘diffraction tomography’, will be used to determine the atomic structure of sub-micron small molecule crystals by acquiring electron diffraction patterns as a function of specimen tilt. Secondly, 4D scanning electron diffraction (4D-SED) will be used to study the heterogeneous microstructure of pharmaceutical material, investigating grain orientation, boundaries and interfaces, and crystal defects - all of which play a role in determining the materials’ properties. This project will focus also on how best to analyse these large multi-dimensional datasets, harnessing digital technologies and developing 'big data' methods of machine learning and artificial intelligence that are optimised for electron diffraction.

The successful candidate would have interests in combining data analysis with experimental electron diffraction. Previous experience in data analysis, using python, and some knowledge of electron microscopy, would be highly desirable. We are looking for candidates interested in collaborative work as the project will involve interacting closely with industrial partners.

Applicants should have (or expected to be awarded) an upper second or first class honours degree at the level of MSci, MEng (or overseas equivalents) in a relevant science subject (e.g. Physics, Chemistry, Materials Science).

EPSRC ICASE studentships are fully-funded (fees and maintenance) for eligible students. A fixed sum of £10,000 per annum for four years (exclusive of VAT) will be paid by GSK to support the Studentship.

This will be used to supplement the annual maintenance (up to £3,000 pa) and support research expenses.

Further details about eligibility and funding can be found at:
https://epsrc.ukri.org/skills/students/help/eligibility/
https://www.postgraduate.study.cam.ac.uk/finance/fees

The PhD will be supervised jointly by Prof Paul Midgley, University of Cambridge, and by Drs Roy Copley and Duncan Johnstone, GSK.

Informal enquiries about this studentship can be made to Prof Paul Midgley at: pam33@cam.ac.uk or to Dr Rosie Ward at: remw2@cam.ac.uk

Applications should be submitted via the University of Cambridge Applicant Portal https://www.postgraduate.study.cam.ac.uk/courses/directory/pcmmpdmsm, with Prof Paul Midgley identified as the potential supervisor. Note that the University charges a £70 fee for PhD applications.

Both the University of Cambridge and GSK are passionate about recruiting the best talent irrespective of their background. We actively support equality, diversity and inclusion and encourage applications from all sections of society.

## PhD Studentship: Computational Design of Resource Efficient Catalysts for Hydrogen Generation

Sponsor: supported by BP through an EPSRC Industrial CASE award. 'Home rate' students
Supervisors: Dr Enrique Galindo-Nava and Prof Manish Chhowalla
Closing date: 31 January 2021

### Project Background

Realising a "Hydrogen economy" is seen as a definite solution to tackle climate change and future energy demands. However, a main challenge for extensive use of hydrogen-based technologies is the sustainable generation of hydrogen through electrocatalytic methods. Platinum remains the preferred catalytic material due to its outstanding electrochemical performance but its very high costs and sluggish kinetics for oxygen reduction have motivated extensive research for suitable substitutes. Although numerous alternatives have been proposed, very few represent a feasible choice for commercial deployment when considering technological requirements such as excellent electrochemical performance, material stability and costs.

This project is aimed at developing a novel computational toolbox to design resource efficient alloy catalysts for hydrogen generation. The toolbox will combine a number of Material Modelling techniques with Data Science to study key features in materials, such as chemical composition, phase fraction and morphology,that control their catalytic activity and stability, whilst minimising additions of precious metals. Thermodynamic modelling will be used to study phase equilibria and stability to identify candidate alloy compositions. Kinetic Monte Carlo will be employed to understand material stability in detail at the atomic-scale. Machine and Deep learning will be used to establish quantitative links between material properties, catalytic activity and electrochemical environments and accelerate the material discovery process. The project will also involve targeted experimental work to validate the models and synthetise newly designed alloys.

The successful candidate would have interests in combining computational modelling with experimental work. Previous experience in Thermodynamic or atomistic modelling is highly desirable. We are looking for candidates interested in collaborative work as the project will involve interacting closely with our industrial partners. The project is suitable for a candidate with background in materials science, engineering, chemistry, applied mathematics or related disciplines.

Applicants should have (or expected to be awarded) an upper second or first class UK honours degree at the level of MSci, MEng (or overseas equivalents) in a relevant science subject (Physics, Chemistry, Materials Science, Mathematics) and should meet the EPSRC criteria for UK/EU residency and liability for 'home rate' fees (https://epsrc.ac.uk/skills/students/help/eligibility/) to be eligible for a studentship.

The on-line application system is available at https://www.graduate.study.cam.ac.uk/. Further information on the application process is available from Rosie Ward (remw2@cam.ac.uk).

Informal enquiries may be made to Dr Enrique Galindo-Nava (eg375@cam.ac.uk) and Professor Manish Chhowalla (mc209@cam.ac.uk).

## PhD Studentship: Resistive switching in oxides

Supervisor: Prof Judith Driscoll https://driscoll.msm.cam.ac.uk/
Sponsor: ERC Advanced Grant, EROS: https://cordis.europa.eu/project/id/882929
Start date: 1st October 2021
Fixed-term: The funds for this post are available for 3.5 years
Closing date: 20 December 2020

The amount of digital information produced globally is exploding. 90 % of the world's data that existed in 2016 had been created in the previous two years alone. Oxide switching materials have promise for non-volatile memory and neuromorphic computing, and could change the technology landscape in artificial intelligence, security, IoT and beyond.

The goal of this ERC Advanced Grant project, EROS, is to undertake research in the area of practical and reliable oxide thin film materials, which display resistive switching effects. The successful applicant should be highly self-motivated, ambitious and show initiative, they will be expected to do experimental research in a team environment working with researchers across departments on device fabrication and characterisation. They should be able to analyse and interpret the results of own research and generate original ideas based on outcomes, design and conduce a coherent set of experiments and record their outcome. They will work under the supervision of Prof Driscoll, and will collaborate with a junior lecturer, postdocs, students, and with two groups in the USA.

A background in Materials Science, Physics, Electrical Engineering, or closely related disciplines is required. The student selected for this project will be trained on thin film growth techniques, and a wide range of materials and electrical characterization tools, join a growing interdisciplinary group. Applicants should have (or expect to be awarded) a first-class or an upper second UK honours degree at the level of MSci, MEng (or overseas equivalent) and should be eligible for 'home rate' fees.

The on-line application system is available at https://www.graduate.study.cam.ac.uk/. Further information on the application process is available from Rosie Ward (remw2@cam.ac.uk).

For more information about this studentship contact Prof Judith Driscoll (jld35@cam.ac.uk).

## PhD Studentship: Nanionic Energy Devices

Supervisor: Professor Judith Driscoll
Sponsor: EPSRC and Cambridge Display Technology (CDT)
Start date: October 2020
Full studentship, available to 'home rate' fee payers only

Applications are invited for a PhD studentship fully funded for a student paying 'home rate' fees, and will run for up to 3.5 years from October 2020. It will be based in the Department of Materials Science and

Metallurgy at the University of Cambridge and will be run in close collaboration with Cambridge Display Technology (CDT) - https://www.cdtltd.co.uk/.

The first grand challenge in the Government's 2017 industrial strategy white paper is, 'put the UK at the forefront of the artificial intelligence and data revolution'. NVM technologies are key to advances in cognitive computing, boosting the development of artificial intelligence. The second grand challenge relates to adoption of energy efficient materials, e.g. batteries, photocatalysts. These systems have in common electrochemical processes.

Controlling and understanding the ionic motion at the nanoscale is critical for performance optimization of the aforementioned energy devices. However, so far, there has been little nanoscale probing undertaken of these processes. There is a real opportunity to advance these widely varying energy technologies by studying model thin film single-crystal-like systems, utilizing new characterization tools to probe model systems of different dimensionalities. Hence, ideal nanoscale films and interfaces will give us an unprecedented opportunity to understand surface vs. bulk processes, and to learn about the influences of strain and defect processes.

**Work to be done**
**Designed nanostructured systems**
We will create single crystal thin films and multilayers using advanced pulsed laser deposition. We will use in-situ XPS to probe chemical and electronic states. We will work with many groups within Cambridge to probe ionic and electronic processes using a combinations of tools in collaboration with Physics, Chemistry, Engineering in Cambridge and teams abroad (e.g. nanoplasmonics, interferometric scattering microscopy, electrochemical AFM, in-operando TEM and NMR).

**Potential Big Wins**
The ability to design and fabricate industrial memristors for memory and AI, which are easy to grow, stable over trillions of cycles, controlled on-off states which can be trained, to fulfil a $Trillion market.
Creating highly stable, high performance solid state batteries
Systems with high rate catalytic processes.

Applicants should have (or expect to be awarded) an upper second or first class UK honours degree at the level of MSci, MEng (or overseas equivalents) and should be should meet the EPSRC criteria for UK/EU residency and liability for 'home rate' fees.

The on-line application system is available at https://www.graduate.study.cam.ac.uk/.
Further information on the application process is available from Rosie Ward (remw2@cam.ac.uk).

## PhD projects for which funding is available from the Department on a competitive basis

## New oxide interface electronics

In the last few years, there have been very exciting reports about the new functional properties which can be achieve at the interface between oxide films, e.g. there is the possibility to achieve new kinds of fast, energy efficient semiconductor processors and even possibly room temperature superconductors. This project involves exploring such phenomena. It will involve growth of ultrathin, single crystal thin films using a world leading, state-of-the-art advanced pulsed laser deposition system with in-situ diagnostic tools (XPS, UPS), followed by their measurement using a variety of means including electrical measurements, synchroton studies, and atomic force microscopy (scanning probe) techniques.

For further information contact Prof J Driscoll (jld35@cam.ac.uk).

Applicants should have (or expect to be awarded) an upper second or first class UK honours degree at the level of MSci, MEng (or overseas equivalents) in a relevant subject (Materials Science, Physics, Chemistry) and should be liable for 'home rate' fees to be eligible for a studentship from the Department.

Other competitive studentship schemes available to overseas fee paying students, deadline 3 December 2019, are described at https://www.graduate.study.cam.ac.uk/finance/funding/graduate-funding-competition.

Applications can be made on-line via http://www.graduate.study.cam.ac.uk/courses/directory/pcmmpdmsm.

Further information on the application process is available from Dr Rosie Ward (remw2@cam.ac.uk).

## Oxide memristors for next generation non-volatile memory in computing

Non-volatile memory (NVM) is critical for all aspects of modern computing, as well in future generation digital technologies like the Internet of Things (IoT) and neuromorphic computing—technologies that will penetrate into many realms of society. Among NVM technologies, resistive random access memory (RRAM) based on metal oxide (MO) films as the resistive switching (RS) layers has the potential of high-speed, low operation voltage, low power consumption, and good endurance that enables the highest performance at the lowest cost possible. There are a number of challenges which need to be addressed with these materials, relating to their nanostructuring and composition. We have solved these problems in a model system and now wish to take this forward to more simple systems. This project will develop such systems. We will collaborate with a number of groups on testing and implementation of industry prototypes.

For further information contact Prof J Driscoll (jld35@cam.ac.uk).

Applicants should have (or expect to be awarded) an upper second or first class UK honours degree at the level of MSci, MEng (or overseas equivalents) in a relevant subject (Materials Science, Physics, Chemistry) and should be liable for 'home rate' fees to be eligible for a studentship from the Department. Other competitive studentship schemes available to overseas fee paying students are described at https://www.graduate.study.cam.ac.uk/finance/funding/graduate-funding-competition.

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Further information on the application process is available from Dr Rosie Ward (remw2@cam.ac.uk).

## Nitride materials and devices for transfer printing and heterogeneous integration

The rapidly developing technique of transfer printing on the micro and nanoscales allows the manufacture of high quality, high performance devices on a wide range of substrates in almost any location. This highly versatile capability features a high-precision mechanical pick-and-place assembly technique that utilises the adhesive properties of soft stamps.  In the context of nitride devices, micro-transfer printing has recently delivered micro-LED arrays that feature in flexible displays and provide inorganic analogues of flexible organic light-emitting diodes (OLEDs) - something that was previously thought to be extremely challenging if not impossible. However, to optimise devices and systems based on transfer printing of nitride materials, it is necessary to both optimise the nitride material for separation from its original substrate and optimise the device design so that its performance is unaffected or even improved by its integration into a heterogeneous system.  This project will explore both the development of materials which allow the transfer printing of a wide range of different nitride devices, both electronic and optoelectronic, and the design of those devices to achieve enhanced performance.

For further information contact Prof RA Oliver (rao28@cam.ac.uk).

Applicants should have (or expect to be awarded) an upper second or first class UK honours degree at the level of MSci, MEng (or overseas equivalents) in a relevant subject (Materials Science, Physics, Chemistry) and should be liable for 'home rate' fees to be eligible for a studentship from the Department.

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Applications can be made on-line via
http://www.graduate.study.cam.ac.uk/courses/directory/pcmmpdmsm.

Further information on the application process is available from Dr Rosie Ward (remw2@cam.ac.uk).

*The University of Cambridge and the Department of Materials Science & Metallurgy value diversity and are committed to equality of opportunity.*