UNIVERSITY of GREENWICH

Information on Postgraduate Research Scholarship - Ref: M34Impact-MSE2			
Faculty:	Engineering and Science	**Department:**	Computing and Mathematical Sciences
Lead Supervisor:	James Le Houx		
Project Title:	The Self-Driving Microscope: Predicting Stochastic Failure in Solid-State Batteries using Physics-Informed AI		
Project Description:	The development of safe, high-energy solid-state batteries is a key UK national priority, but it faces a critical bottleneck: the microscopic flaws that cause catastrophic failure (such as dendrite penetration, severe structural cracking, and short-circuiting) are unpredictable, fleeting, and hidden from standard tests. Capturing these elusive, stochastic events is a recognised 'grand challenge' for scientists. This PhD studentship is the foundational computational element (WP1) proposed for a major 8-year project ("The Self-Driving Microscope"). The project's goal is to build an autonomous, AI-piloted X-ray imaging platform that intelligently hunts for these hidden failure points in real-time. As the first PhD student and a founding member of the new BASE (Beamlines for Autonomous Science and Engineering) Laboratory, your goal is to design and build the core predictive engine for this platform, teaching microscopes how to think and helping develop the next generation of beamlines. This is a cutting-edge computational project at the intersection of AI, physics-based simulation, and materials science. Your key objectives will be to: • Build a Multi-Scale Training Dataset - You will use 3D X-ray tomograms of next-generation solid-state cells (e.g., Li-metal/Li_6PS_5Cl) acquired at the I13-2 beamline (Diamond Light Source). The dataset will capture cells at pristine, aged, and post-failure stages. • Develop the Core AI Predictor - You will explore and train advanced models, such as Graph Neural Networks (GNNs), to solve the key challenge: distinguishing benign aging from true failure precursors, features retrospectively confirmed to be the origin of a crack. • Integrate Physics-Based Signatures - You will go beyond simple image recognition by using high-performance computing solvers (like the open-source OpenImpala developed by our group) to transform static 3D porosity maps into dynamic 3D maps of local tortuosity and ionic flux. This provides a direct, physically-grounded signature for the AI to learn from. • Augment Data with Generative AI - You will use physics-constrained generative models (Diffusion models/GANs) to		

	create a diverse library of synthetic microstructures, improving model generalisation against noisy, live experimental data. This studentship is fully and securely funded by the University's £9M Research England-funded M^{3}4Impact expansion programme. This project is a cornerstone of the Computational Science and Engineering Group's (CSEG) goals and will proceed as a key foundational project for the new BASE Laboratory. You will be fully embedded within the M^{3}4Impact doctoral cohort and co-supervised by Prof. Andrew Kao, whose group will provide validated simulation models to benchmark the AI's prediction and Dr. Mikhail Poluektov. As the founding PhD student of the new BASE Laboratory, the successful applicant will join a dynamic, growing research group. The lab is structured with a computational core at the University of Greenwich and an experimental hub at the Rutherford Appleton Laboratory (RAL). Your supervisor, Dr James Le Houx, is the Faraday Institution Emerging Leader Fellow at RAL and co-leads the UK's Battery Imaging BAG at Diamond Light Source. You will benefit from this direct link to national facilities and be part of a team dedicated to developing open-source computational tools for advanced materials discovery.
Duration:	4 years, Full-Time Study or 7 years, Part-Time Study

Bursary available (subject to satisfactory performance):
Rates below are for full time (FT) mode.
Year 1: £24,780 (£20,780 UKRI rate + London weighting = £2,000 + Enhanced bursary = £2,000)
Year 2: In line with UKRI rate + London weighting = £2,000 + Enhanced bursary = £2,000
Year 3: In line with UKRI rate + London weighting = £2,000 + Enhanced bursary = £2,000
Year 4*: In line with UKRI rate + London weighting = £2,000 + Enhanced bursary = £2,000

In addition, the successful candidate will receive a contribution to tuition fees, equivalent to the University Home Rate, currently £5, 006 (FT), for the duration of their scholarship. International applicants may need to pay the remainder tuition fee for the duration of their scholarship**.

This fee is subject to an annual increase.

* The bursary is for 3 years with a potential extension of up to a maximum of 12 months. Funding extensions may be granted if the student demonstrates, to the satisfaction of the M^{3}4Impact Principal Investigators and PhD supervisors, that the thesis can be completed during the granted extension period.
** For exceptional international applicants the tuition fees may be covered by the M^{3}4Impact

Person Specification of Essential (E) or Desirable (D) requirements:

Criteria:	**E or D**
Education and Training:	
• 1st Class or 2nd class, First Division (Upper Second Class) honours degree or a taught master's degree with a minimum average of 60% in all areas of assessment (UK or UK equivalent) in a relevant area (e.g., Computer Science, Physics, Materials Science, Engineering) or equivalent professional experience.	E
• For those whose first language is not English and/or if from a country where English is not the majority spoken language (as recognised by the UKBA), a	E

language proficiency score of at least IELTS 6.5 (in all elements of the test) or an equivalent UK VISA and Immigration secure English Language Test is required, if your programme falls within the faculty of Engineering and Science a language proficiency score of at least IELTS 6.5 overall with a minimum of 6.0 in all elements of the test or an equivalent UK VISA and Immigration secure English Language Test is required. Unless the degree above was taught in English and obtained in a majority English speaking country, e.g. UK, USA, Australia, New Zealand, etc, as recognised by the UKBA.	
Experience & Skills:	
• Previous experience of undertaking research (e.g., undergraduate or taught master's dissertation).	E
• Strong programming skills in Python.	E
• A high motivation to learn new technical skills in machine learning and data science.	E
• Experience with machine learning, deep learning (e.g., CNNs, GNNs, GANs), or computer vision.	D
• Experience with 3D image data (e.g., X-ray computed tomography) or scientific data analysis.	D
• Experience with physics-based simulation (e.g., CFD, FEA) or high-performance computing (HPC).	D
Personal Attributes:	
• Strong personal motivation and resilience, with a clear understanding of the self-directed nature of a research degree.	E
• An ability to work independently, take ownership of a long-term project, and make consistent progress.	E
• A genuine curiosity and enthusiasm for collaborative, interdisciplinary science.	E
• Experience or interest in contributing to new projects, workflows, or open-source tools.	D
Other Requirements:	
• This scholarship may require Academic Technology Approval Scheme (ATAS) approval for the successful candidate if from outside of the EU/EEA.	E
• The scholarship must commence by 01 September 2026.	E
Closing date for applications:	***midnight UTC on 17th April 2026***
For further information contact:	**Dr James Le Houx (james.lehoux@gre.ac.uk)**

Making an application:

Please read this information before making an application.

All applications **must include** the following information. **Applications not containing these documents will not be considered.**

- **Scholarship Reference Number ("M34Impact-MSE2")**– included in the personal statement section together with your personal statement as to why you are applying
- **a CV including 2 referees** *
- **academic qualification certificates/transcripts and IELTs/English Language certificate if you are an international applicant or if English is not your first language or you are from a country where English is not the majority spoken language as defined by the UK Border Agency** *

**upload to the qualification section of the application form. Attachments must be a PDF format.*

Before submitting your application, you are encouraged to liaise with the Lead Supervisor on the details above.

Information on the application process is available at: https://www.gre.ac.uk/research/study/apply/application-process. Applications need to be made online via this link. **No other form of application will be considered**.