

## Exciting [Faraday Undergraduate Summer Experience \(FUSE\)](#) paid internship opportunities for summer 2023

Studying a STEM degree? Wondering what career to pursue? Interested in finding out more about the battery sector? Keen to spend time with a dynamic community of pioneering battery researchers seeking to find solutions to support a fully electric future?

The Faraday Institution is offering a total of 55 internships, for undergraduate students to spend 8-weeks working on battery related projects.

### Project title

Theoretical spectroscopy to investigate degradation in NMC cathodes

### Project description

$\text{Li}_x\text{Ni}_{1-y-z}\text{Co}_y\text{Mn}_z\text{O}_2$  (NMC) are layered transition-metal (TM) oxides and excellent cathode materials due to high energy densities. At high voltages and temperatures, they are susceptible to oxygen loss, evolution of reactive singlet oxygen ( $^1\text{O}_2$ ) which degrades these cathodes. Studying the evolution of XAS TM edges as a function of states-of-charge (SoC) provides insight into mechanisms of degradation. Accurate modelling of TM edges obtained from experiments in single particle Density Functional Theory (DFT) is difficult and ab-initio multiple scattering (AIMS) methods based on Green's functions is an effective method to model TM XANES edges. In this project, we shall explore the XAS TM edges of NMCs with varying Ni content at various SoC with ab-initio multiple scattering method based on GW approximation, focusing particularly on how the SoC influences the oxidation states of TM which is expected to lead to an understanding of the emergence of excited states like  $^1\text{O}_2$ , as well as explain relative stabilities of NMCs with varying Ni content.

### Project Goals

In conducting the project, you will gain a wider knowledge of lithium-ion battery degradation. You will learn the basics of performing first principles electronic structure calculations using DFT and AIMS codes like Feff. Feff is an easy to use code suitable for undergraduates and can be of use for theorists and experimentalists alike. You will have an introduction to some of the state-of-the-art many body theory methods like GW approximation, Random Phase approximation etc in solid state physics.

As part of the project you will be supported by leading academics to develop skills in simulation and analysis of data which underpins the performance and degradation of NMC cathodes. Throughout the project you will develop your research skills while working in a team comprising of both theorists and experimentalists in this exciting area.

**Supervisor** Dr. Hrishit Banerjee, in the group of Prof Dame Clare Grey

**University** University of Cambridge

**Location** In-person, in Cambridge

**Start date** The internship is a full-time role for eight weeks between June – September 2023

### Eligibility

- Be registered full-time undergraduate student from a UK university.
- Undertake the internship within the years of their undergraduate study (i.e., not in final year or during a subsequent Masters' programme).
- Not have been a FUSE intern in a previous year

## **Funding**

A salary of £10.90/ hour across the UK or £11.95 / hour in London will be provided. This will be determined by the working address of the appointee, not the university's location. The funding is provided by the [Faraday Institution](#).

## **Additional activities**

During the FUSE internship you will be able to attend Faraday Institution cohort events which will focus on a variety of topics to further develop your understanding of career opportunities in battery sector. At the end of the programme, you will be invited to share a poster about your work and prizes will be awarded.

## **Application**

To apply, please complete this [survey](#) by 23.59 on 17 April 2023.

For project information, please visit <https://faraday.ac.uk/research/lithium-ion/extending-battery-life/>

## **Diversity**

The Faraday Institution is committed to creating a dynamic and diverse pool of talent for the fields of battery technology and energy storage.

The University of Cambridge is committed in its pursuit of academic excellence to equality of opportunity and to a pro-active and inclusive approach to equality, which supports and encourages all under-represented groups, promotes an inclusive culture, and values diversity.