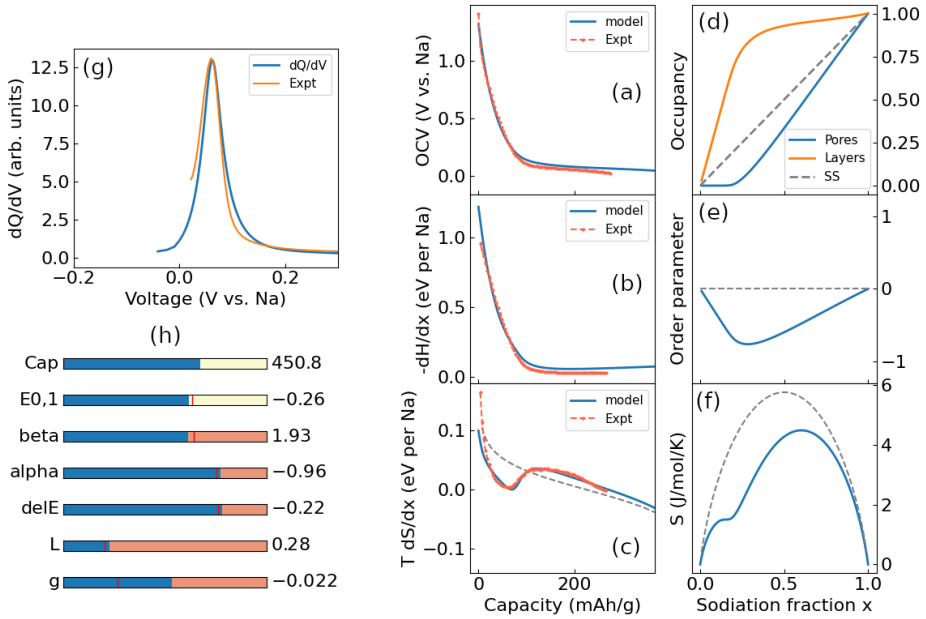
THE FARADAY INSTITUTION Modelling
MULTI-SCALE MODELLING

Thermodynamic measurement of sodium in hard carbons

Project Description

Hard carbon is the most promising anode material for sodium-ion batteries [1, references below], a possible alternative to lithium ion batteries using cheaper and more abundant sodium. However, the working principles of sodium insertion/removal between layers and in pores lack comprehensive understanding, causing challenges in cell control and commercialisation.

Unpublished data (**Figure**) show measurements (red lines, a-c) from sodium insertion into one hard carbon sample compared with models (adapted from [2,3], blue lines), via an interactive tool, allowing the measured behaviour to be modelled with adjustable input parameters (h). More information than just the measured cell voltage (a) allows pore and layer sodium occupations to be determined (d).



Project Goal

You will perform experimental entropy characterisation [2] on a wider range of already synthesised hard carbon samples from collaborators [1] and obtain model parameters by fitting the experimental results via the interactive tool. In this way, better understanding of the pore versus layer contributions will be obtained dependent on hard carbon morphology. By joining our diverse team in Energy Lancaster, you will be contributing by using our novel experimental characterisation and modelling methodologies to support materials research, control systems, and quality control in production.

We are closely montoring the ongoing COVID situation and the current plan is for the project to be partly lab-based, which would require the intern to be in Lancaster for the duration of the project. In

the event that lockdown restrictions prevent this over the summer, the project will switch to fully computational and will run remotely.

FUSE students will invited to participate in a Faraday Institution event to share their posters with UK battery researchers and industry partners. Prizes will be awarded.

Eligibility

In order to partake in the project you must be:

- A full-time registered undergraduate student at a UK university
- Undertake the internship within the years of undergraduate study (i.e. not be currently in your final year)

Lancaster University provides a research environment that strongly supports the individual needs of each staff member and promotes a healthy work-life balance. We are committed to the Athena Swan Charter, which recognises and celebrates good employment practice undertaken to address gender equality in higher education and research. Our commitment to these principles is reflected in our recent receipt of an Athena Swan Bronze Award.

Funding

A salary of £9.50/hour across the UK or £10.85/hour in London will be provided. This will be determined by the working address of the appointee, not the university's location. The internship is a full-time role for 8 weeks beginning in June-early July. The funding is provided by The Faraday Institution.

Please send your CV and a brief cover letter to m.mercer1@lancaster.ac.uk by 7th May 2021.

The criteria for selection will be:

Essential: a clear rationale for applying for the position and how it fits with the candidate's career goals.

Essential: evidence of interest and motivation for the research area.

Essential: some experience in a high level programming language, preferably Python.

Essential: ability to document work done and flexibility to discuss slides on ongoing results of the project with the supervisor weekly, and update the supervisor promptly on any challenges faced.

Desirable: experience in battery, coin cell, or experimental electrochemical characterisation.

Desirable: knowledge of statistical thermodynamics.

Related papers and further reading

[1] "A revised mechanistic model for sodium insertion in hard carbons", *Energy and Environmental Science* **13** (2020) 3469-3479

[2] "Transitions of lithium occupation in graphite: A physically informed model in the dilute lithium occupation limit supported by electrochemical and thermodynamic measurements", *Electrochim. Acta* **324** (2019) 134774.

[3] "Voltage hysteresis during lithiation/delithiation of graphite associated with meta-stable carbon stackings", *J. Mater. Chem A* **9** (2021) 492-504