THE FARADAY INSTITUTION LiSTAR
NEXT GENERATION LITHIUM SULFUR BATTERIES

The University of Nottingham

Thiolated Quinones as Redox Mediators

Project Description

Accelerating the conversion of S to Li_2S is a critical challenge hindering development of the lithium-sulfur battery. Quinone-based redox mediators are promising homogenous catalysts for conversion between S and Li_2S, enhancing rate and capacity performance. However, redox potentials of typical quinones are not ideally placed for deep discharge of lithium-sulfur cells. Here we propose a new set of redox mediators based on thiolated quinones, which are expected to operate at moderate potentials and show increased stability of the radical intermediate. Quantum chemical calculations will be performed to study the interaction of S with thiolated di-tert-butyl quinones to determine the relative stability of the radical intermediates. Output from the calculations will help direct future experimental work where the best candidates of thiolated di-tert-butyl quinone based mediators, from the molecular modelling, will be synthesized and their electrochemical properties in battery-relevant electrolyte solutions will be determined.

Due to the ongoing COVID-19 situation, the entire project will be running remotely, unless the existing restrictions are removed.

Project Goals

In conducting the project, you will gain a wider knowledge of the lithium-sulfur battery and develop skills applicable to computational chemistry, with a focus on high-performance computing skills. You will be supported by leading academics to generate, process and analyse output from molecular modelling, and gain experience working in a research environment. As part of the project, you will be given the opportunity to enter a poster competition to present your work at the Faraday Institution Conference in November 2020.

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)

Funding

A salary of £9.30/hour across the UK or £10.75/hour in London will be provided. This will be determined by the working address of the appointee not the universities location. The internship is a full-time role for 8 weeks beginning in early July. The funding is provided by The Faraday Institution.

Deadline

Please send you CV and a brief cover letter to david.rogers@nottingham.ac.uk by June 1st

For project information, please visit www.listar.ac.uk