Density functional theory investigation of Redox flow battery electrolytes

Project Description

Flow batteries are a promising technology for grid-level storage of energy. However, to improve their performance, new electrolytes need to be designed and tested. Within this remit, organic electrolytes are growing to be a promising category. Moreover, the positive redox couple, i.e. the catholyte or posolyte, proves to be a tricky field of investigation. However, there are currently few viable water-soluble posolytes that have the necessary solubility or electrochemical stability to be used in a flow battery system. The project involves the use of density functional theory (DFT) calculations to assess the viability of new flow battery electrolytes. The student will require a working internet connection and their own personal computer to access the computer cluster on which the calculations will be run. Key target properties will include the molecular redox potential and its interactions with water. To aid in future characterisation, spectral properties such as NMR, EPR, UV-Vis and IR will also be investigated to elucidate promising candidates for synthesis and further investigation.

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

Project Goals

The project will allow you to pick up and improve your command line shell/Bash skills alongside developing a familiarity with molecular DFT. Through modelling of solvation interactions, redox reactions, and spectral properties such as NMR, EPR, UV-Vis and IR interesting candidates for further synthesis and investigation will be identified. Electrolyte design and stability is critical for flow battery performance and development. Through the project, you will gain a wider knowledge of flow batteries and develop your research skills while working alongside leading academics in this exciting area.

As part of The Faraday Institution's 2020 intern cohort you will enter an end-of-project poster competition – the winners of which will be invited to present their poster 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 your two page CV and a no more than one page cover letter to sm2383@cam.ac.uk by 8 June.

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