

## Molecular modelling of lithium-ion diffusion through a polymer layer

### Project Description

This project is under the umbrella of the LiSTAR project, a Faraday-funded project on Lithium-Sulphur (Li-S) batteries. Shuttling of polysulphides between cathode and anode is a major problem in Li-S batteries, reducing battery capacity and lifetime, while it also affects the lithium (Li) anode via undesired reactions of the sulphides at the anode surface. Polymer layers may be used to protect the Li-anode and also as solid polymer electrolyte. However, the slow diffusion of  $\text{Li}^+$  ions through these solid layers reduces the power density and even the energy density of the battery. For this reason, special polymers are designed to facilitate  $\text{Li}^+$  ion diffusion while they still retain their solid state. The aim of this project is to use molecular modelling and simulations to assess different polymers.

The FUSE intern, supported by researchers at the University of Surrey, will create polymer models using software such as PACKMOL, for different polymers, polymer blends and copolymers proposed by the academic supervisor. Molecular dynamics (MD) simulations will be employed to determine the diffusion coefficient of  $\text{Li}^+$  ions through these polymers.

***Due to the ongoing COVID-19 situation, the entire project will be running remotely.***

### Project Goals

Join the Faraday Undergraduate Summer Experience (FUSE) internship programme and learn more about the art of designing materials via molecular modelling which will help in the development of a career in the field of battery technology and energy storage. In conducting the project, you will develop skills in the use of molecular modelling software such as PACKMOL and Materials Studio. You will also be trained in writing scripts and running jobs using MD software such as Gromacs on the Higher Performance Computers at the University of Surrey.

### Eligibility

In order to partake in the project you must be:

- A full-time registered undergraduate student at a UK university, studying Chemistry, Physics, or Materials Science and Engineering.
- Undertake the internship within the years of undergraduate study (i.e. not be currently in your final year)

### 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 universities location. The internship is a full-time role for 6-8 weeks beginning in June-early July. The funding is provided by [The Faraday Institution](#).

### Deadline

Please send you CV and a brief cover letter to Professor Constantina Lekakou [c.lekakou@surrey.ac.uk](mailto:c.lekakou@surrey.ac.uk) by 30 April 2021.