

## Molecular-level simulations for the predictions of Li-ion diffusivity through solid sulphur and solid sulphides

### 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. The latest cathodes under research are composites of sulphur impregnated in a porous carbon scaffold. In designing the pore size distribution of this scaffold, it has been speculated that small micropores could hold the sulphur and subsequently generated sulphides and, thus, reduce the “shuttling” effect. The question is then if  $\text{Li}^+$  ions can diffuse through the solid sulphur or sulfur softened by the electrolyte solvents, and how fast this diffusion might be. The aim of this project is to employ molecular simulations to investigate the diffusion of  $\text{Li}^+$  ions through solid or solvent-softened sulphur.

The FUSE intern, supported by researchers at the University of Surrey, will create sulphur and solvent-sulphur models using software such as AVOCADRO or PACKMOL. DFT simulations will be then employed to determine the diffusion coefficient of  $\text{Li}^+$  ions.

***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 using 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 Avocado, PACKMOL and Materials Studio. You will also be trained in writing scripts and running jobs 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.