LONDON'S GLOBAL UNIVERSITY

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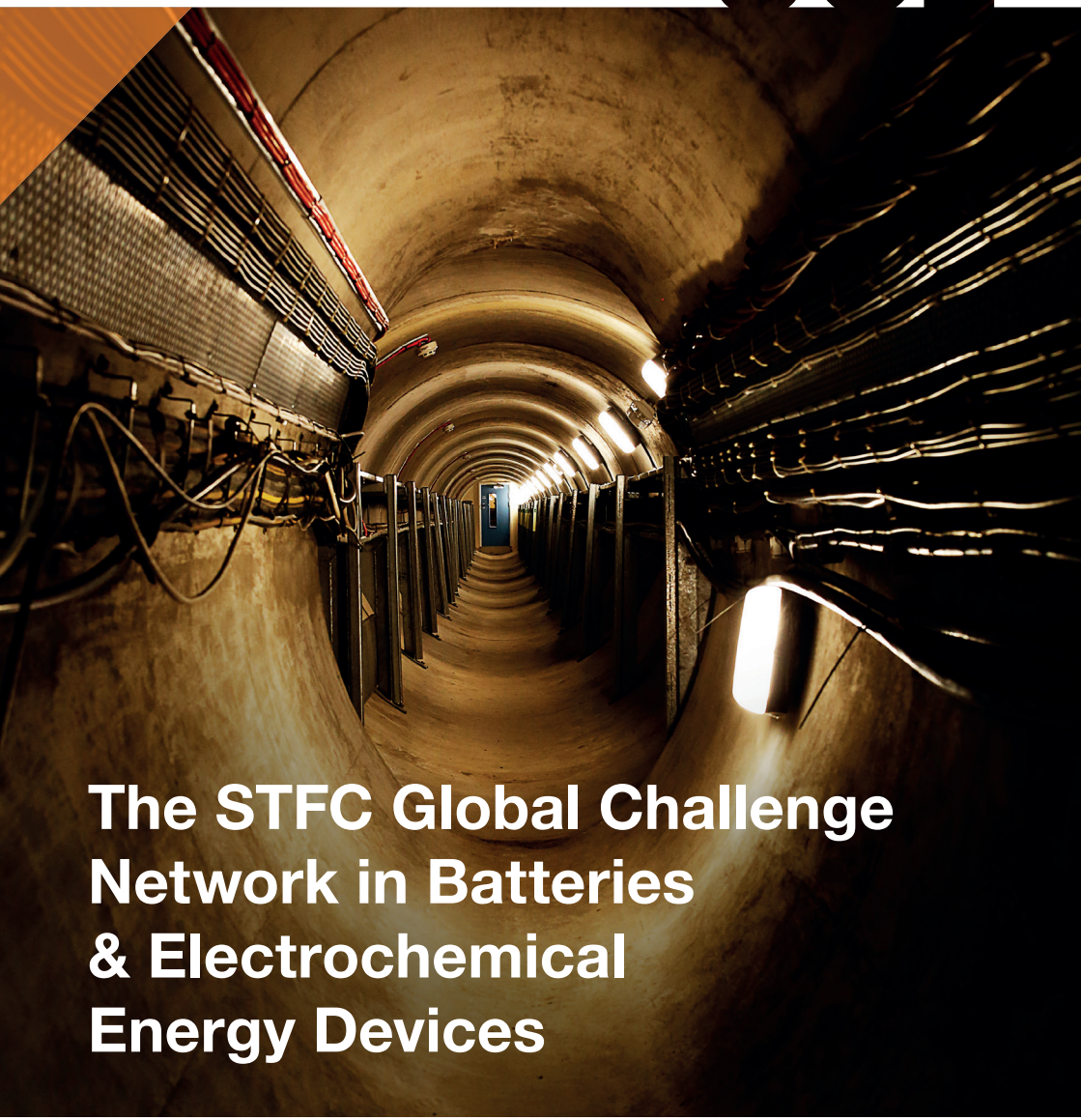

The STFC Global Challenge Network in Batteries & Electrochemical Energy Devices

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Change the world

Science & Technology Facilities Council

Introduction

The STFC Global Challenge Network in Batteries and Electrochemical Energy Devices, brings together leading researchers in industry and academia with a shared interest in the application of large-scale user facilities, to address key challenges in battery science and technology.

Large scale user facilities play a pivotal role in the development of new and improved electrochemical energy devices including batteries and fuel cells.

The Network will promote collaboration between world-class users and developers of large-scale research facilities and provide a forum to draw together researchers from a range of disciplines. Network members are encouraged to share latest technique developments and help disseminate cutting-edge research ahead of publication. This is achieved through targeted network events.

Membership of the Network is open to all stakeholders with an interest in the application of large-scale facilities – access to associated funding is reviewed by the Network's steering committee.

The objectives of the Network are:

1. Bringing together an international community of researchers from industry, academia and national laboratories.
2. Seeding lasting collaborations which will lead to cutting edge science.
3. Establishing cross-technique linking between different users of large-scale facilities.
4. Standardising new techniques (especially for applications to electrochemical devices).
5. Establishing and disseminating best-practice methodologies.
6. Ensuring best use of large-scale facilities resources and complementary science.
7. Providing advice and feedback to inform future infrastructure investment.
8. Promote the engagement of industry with large scale facilities.

Events

The Network supports a range of events, which are free to all to attend including:

- Annual scientific meetings
- Annual early-career researchers' meetings
- Industry workshops
- Early-career training workshops and summer schools
- Technique development workshops
- Fieldtrips to synchrotron and neutron sources

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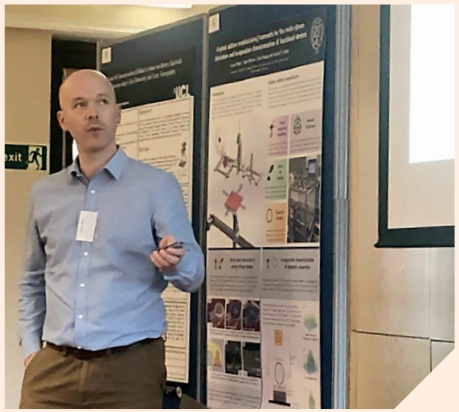
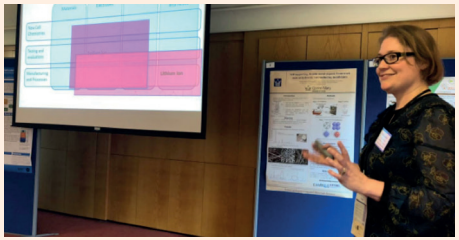
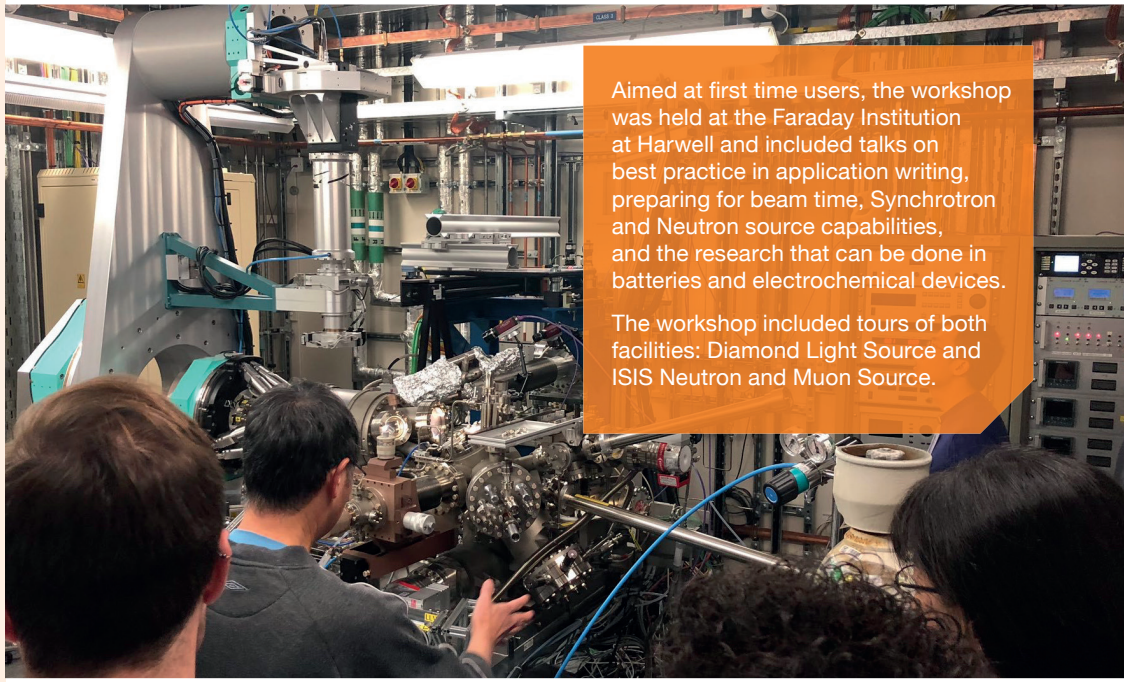
Early Career Researchers' Meeting



Hosted at The Cosener's House, Abingdon, the two-day Early Career Researchers' Meeting continues to provide an opportunity for those in the early stages of their research career, PhDs and Post-Docs, to present and discuss their work in a relaxing environment and creating links and collaborations. The meeting also included four senior keynote speakers presenting their recent research in the fields of batteries, fuel cells and other electrochemical applications; as well as an Industry Speed Dating afternoon.

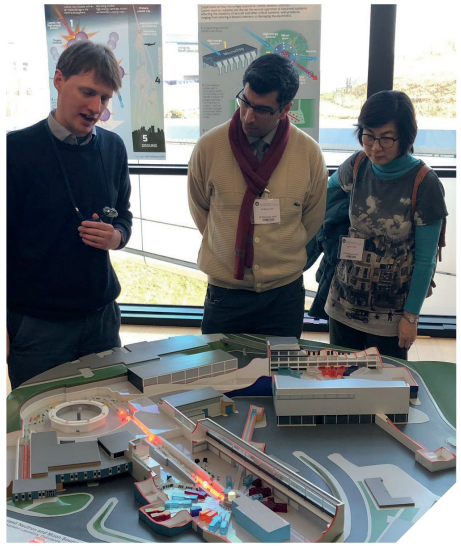


Beam-Time Application Workshop

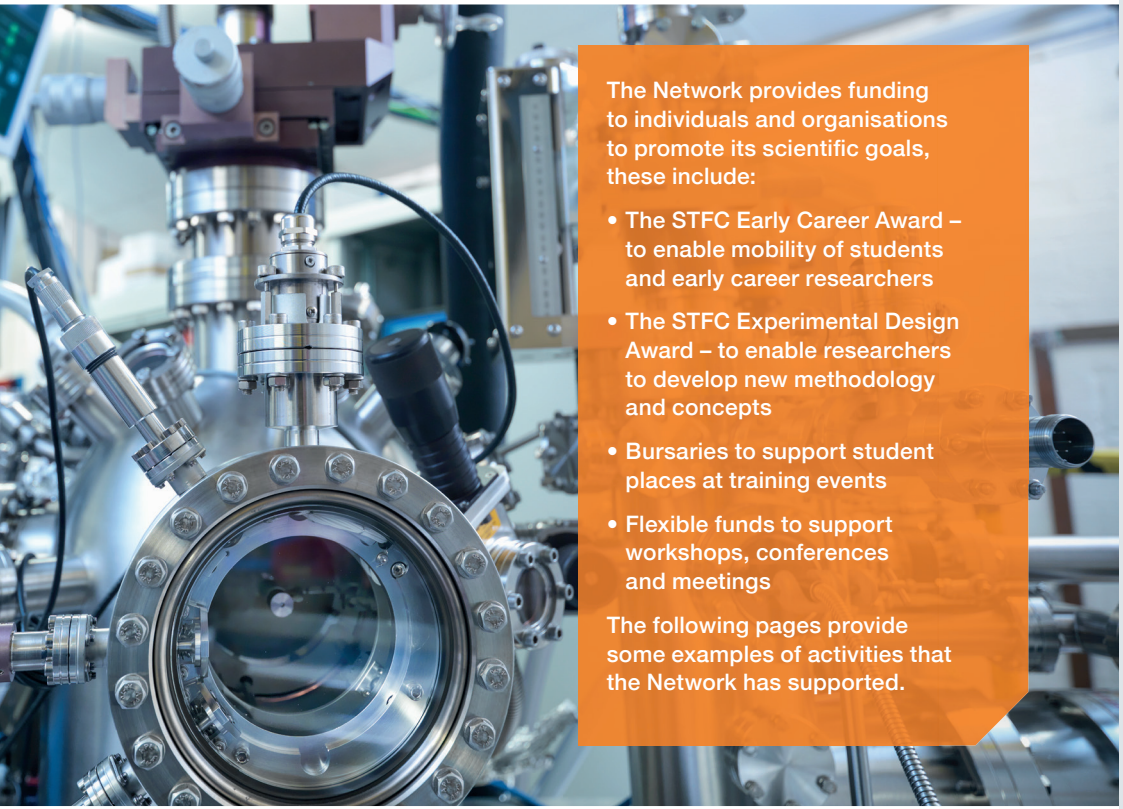


Aimed at first time users, the workshop was held at the Faraday Institution at Harwell and included talks on best practice in application writing, preparing for beam time, Synchrotron and Neutron source capabilities, and the research that can be done in batteries and electrochemical devices.

The workshop included tours of both facilities: Diamond Light Source and ISIS Neutron and Muon Source.



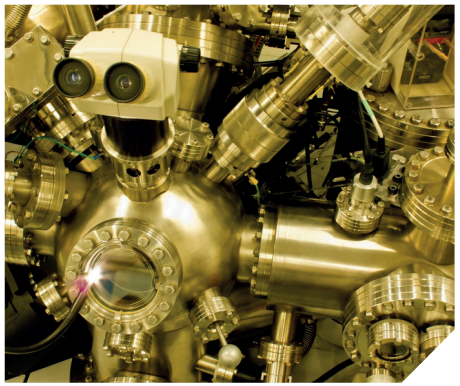
Funding

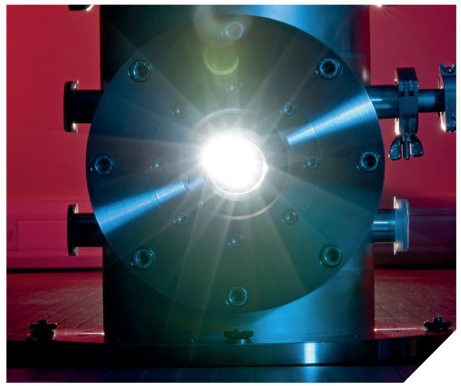


The Network provides funding to individuals and organisations to promote its scientific goals, these include:

- The STFC Early Career Award – to enable mobility of students and early career researchers
- The STFC Experimental Design Award – to enable researchers to develop new methodology and concepts
- Bursaries to support student places at training events
- Flexible funds to support workshops, conferences and meetings

The following pages provide some examples of activities that the Network has supported.

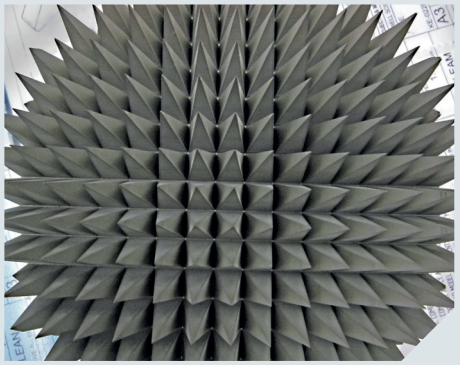




Experimental Design Awards

10 experimental design awards were funded in Phase 2, enabling the development of new research capability in the UK, including:

- Dr Oliver Pecher (University of Cambridge): who, alongside beam line I11 staff, has developed a new high-temperature XRD cell for long duration battery experiments which is yielding insight into the degradation of Li-ion battery materials, leveraging Diamond's unique Long Duration Experiments beamline.
- Dr Julia Parker (Diamond): who is developing a novel electrochemical cell *(see Figure)* for incorporation into the I14 beamline for a range of electrochemical studies.
- Dr Paddy Cullen (UCL/ISIS): who has developed an in-situ environment for battery studies using neutron scattering and diffraction, which will be made available to the wider neutron user community.



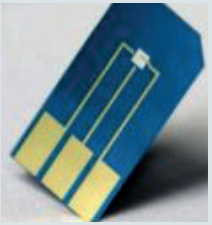


Figure: New hardware developed through the Network's Experimental Design scheme is enhancing UK research capability.

STFC Experimental Design Award

Case Study: Identifying the risks of Li ion battery failure

Dr Donal Finegan – National Renewable Energy Laboratories (NREL)

This project aimed to link internal phenomena that occur during catastrophic failure of Li ion batteries with external risks. The project involved design of in-situ containment vessels that facilitated simultaneous X-ray imaging, thermal imaging, and heat measurements, from commercial Li ion batteries as they undergo thermal runaway. The containment vessels were constructed using the STFC design award and have been utilized at the ESRF and Diamond Light Source for experiments that have since significantly advanced our understanding of the mechanisms that lead to failure of Li ion cells.

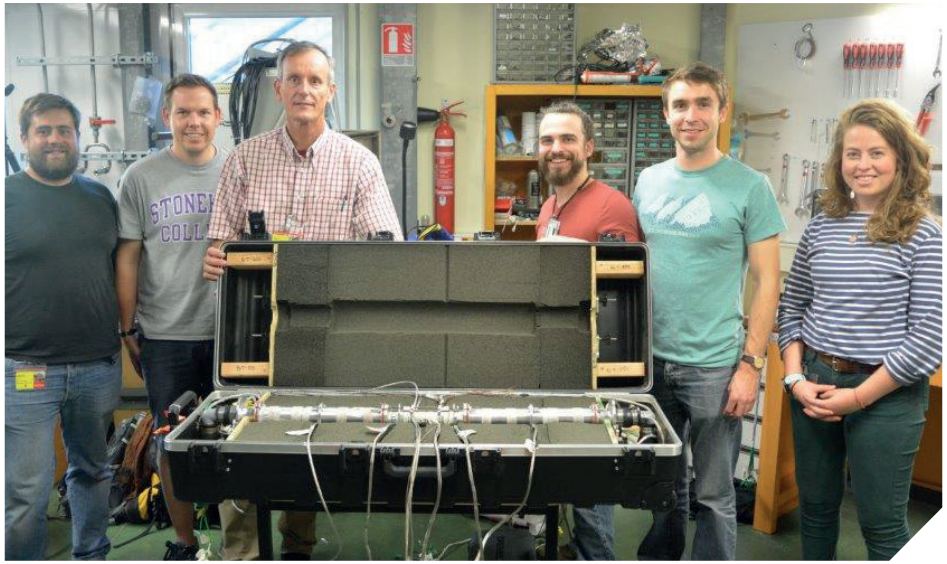
This work attracted the attention of NASA and the US DOE's National Renewable Energy Laboratory (NREL), where I now work.

The award directly contributed to improving my post-PhD career opportunities, continuing my research pursuits at NREL, and for bringing international recognition to the advanced X-ray diagnostic capabilities of the ESRF and Diamond Light Source.

We have since received funding from NASA to further explore the relationship between internal dynamics and external risks for Li ion batteries.

The funding has led to the following publications:

1. Finegan, Donal P., et al. "Modelling and experiments to identify high-risk failure scenarios for testing the safety of lithium-ion cells." Journal of Power Sources 417 (2019): 29-41.
2. Finegan, Donal P., et al. "Identifying the Cause of Rupture of Li-Ion Batteries during Thermal Runaway." Advanced Science5.1 (2018): 1700369.
3. Finegan, Donal P., et al. "Tracking Internal Temperature and Structural Dynamics during Nail Penetration of Lithium-Ion Cells." Journal of The Electrochemical Society 164.13 (2017): A3285-A3291.



Case Study 2

STFC Experimental Design Award

Case Study: In-situ electrochemical XPS

Dr Alex Walton – University of Manchester

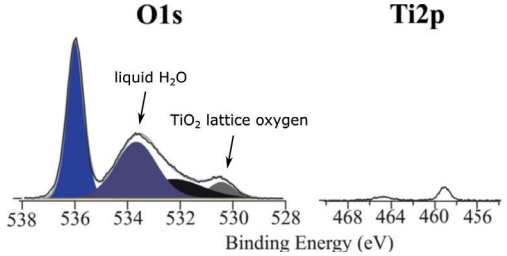
This funding allowed me to develop a new methodology to study the electrode/electrolyte interface in XPS. This would allow operando XPS of electrochemical systems (battery electrolytes amongst others), but is highly technically challenging.

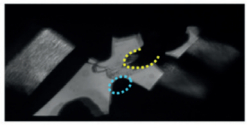
The development was done using our lab-source NAP-XPS instrument in Manchester but with a view to rolling out the same methodology at Diamond (B07 beamline). This rollout is still ongoing.

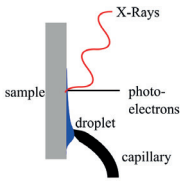
The proof-of-concept paper and follow-on funding resulting from this award has raised my profile, led to a number of new collaborations and to receiving an EPSRC New Investigator Award EP/S004335/1.

The funding has led to the following publication:

Booth, S. G., et al. "The offset droplet: a new methodology for studying the solid/water interface using x-ray photoelectron spectroscopy." Journal of Physics: Condensed Matter 29.45 (2017): 454001.







Case Study 3

STFC Experimental Design Award

Case Study: Design of an electrochemical cell for in-situ spectroscopy

Dr Rosa Arrigo – University of Salford

The aim of the project was the development of an in-situ electrochemical cell for investigating electro-catalytic processes by means of synchrotron based hard X-ray absorption spectroscopy at the synchrotron facility DLS.

Using this in-situ cell, I was able to gain new insights into the electro-catalytic reduction of carbon dioxide over FeOOH supported on C electro-catalysts.

In a previous study, I found that the reactivity of Fe oxides can be tuned by the interaction with the carbon support such that it catalyses the C-C coupling, which is one of the biggest challenges in carbon dioxide reduction. Through this work, it was possible to clarify that Fe(II) sites coordinated to N-functionalities on the carbon support are responsible for the C-C coupling. Moreover, it was possible to identify that the structural transformation of FeOOH species into metallic Fe leads to the parasitic hydrogen evolution reaction. This is a major scientific breakthrough, which was published recently (R. Arrigo, Nature Communication 2018), and the research is still ongoing and other publications are in preparation.

This award enabled me to engage with the wider UK scientific community to study in-situ electro-catalytic processes, specifically with the following institutions:

a) UCL to study ORR over Pt based electrodes;

b) University of Bath and Cardiff and the MAXNet to study the OER over IrOx;

c) University of Oxford to study single metal sites graphene-based electrode for HER and NH3 synthesis.

The funding has led to the following publication:

Genovese, Chiara, et al. "Operando spectroscopy study of the carbon dioxide electro-reduction by iron species on nitrogen-doped carbon." Nature communications 9.1 (2018): 935.

Early Career Awards

The awards programme was established to promote researcher mobility, and to strengthen ties between UK universities and facilities and their international counterparts.

For example:

- Quentin Meyer (UCL), was able to fund himself and three colleagues to travel and stay at the Swiss Light Source, which resulted in three publications in peer-reviewed journals. The funds allowed him and a small team to study the effect of water on an open cathode fuel cell using neutron imaging.
- Pablo Aparicio Sanchez (Cardiff University) was funded to spend time with an experimental group in Singapore to test his theoretical calculations on new active materials for alkali-metal ion batteries experimentally, using facilities that would otherwise be unavailable to him.
- Ian Johnson (UCL) was able to travel and spend one month at the University of Illinois, where he tested materials developed at UCL on Mg-ion batteries used at Illinois.
- Simon Engelke (University of Cambridge) was able to travel to Japan to meet with industry leaders to investigate how the techniques he has developed at Cambridge for synthesising hierarchical electrodes for Li-ion and Li-air batteries could be scaled up in an industry setting, and he has forged links with a Japanese battery research company where he will be undertaking an internship.
- Weixin Song (Imperial College) used the award to fund his travel to other institutes for experimental and analytical work necessary for understanding and improving the performance of graphene in Li-ion batteries which resulted in two publications.

Case Study 4

STFC Early Career Travel Award

Case Study: Implications of structural inhomogeneities and manufacturing defects in carbon fiber-based papers and felts used in energy conversion and storage electrochemical devices

Dr Pablo Angel Garcia-Salaberri – University Carlos III of Madrid

This project is designed to strengthen a nascent collaboration between the two groups in the UK and Spain (and, in particular, between Dr. García-Salaberri and Dr. Jervis who are at an early stage in their independent research careers), with a view to providing proof of concept data for a larger ERC proposal in the future. Improving the fundamental research into the imaging and modelling of electrochemical devices is vital to the UK's future as a green economy, particularly improving grid-scale storage solutions that will allow the expansion of widely available but intermittent wind power in the UK. The combination of leading computational modelling and expertise in imaging of electrochemical systems at UCL will further our understanding of the operation of these devices on the microscale and accelerate their commercial uptake.

The funding allowed me to spend time at the Electrochemical Innovation Lab at UCL and to establish a working relationship with them, resulting in several papers and a potential research project application.

Case Study 5

STFC Early Career Travel Award

Case Study: Unlocking Value of V2G Through SOH Prognostics

Dr Kotub Uddin – Ovo Energy

The funds were used to travel to Singapore for planned meetings at NTU's Energy Research Institute. We collected commercial battery degradation data which we used to develop an LSTM numeral network model for Lithium ion Battery SOH prognostics. We are still working on developing some parts of the model, because we want to assess the models learning capability.

Our experience collaborating with NTU was positive. We are currently exploring:

1. Mechanisms of providing funding for UK based research in energy storage – currently in discussions with a UK HE Institution;
2. Opportunities to invest in new energy storage technologies worldwide.

Notes

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