



Job Ref: REQ211323

Job title: Battery Materials Modelling Research Scientist (KTP Associate)

Period: 24 months

Salary: £30,000 - £40,000 per annum (Starting salary to be confirmed on offer of appointment)

Application deadline: Wednesday 1 December 2021

Key words: Materials science, Chemistry, Materials modelling, Electrochemistry performance

Project Title:

Applying materials modelling approaches to improve the performance of existing active anode material products for next generation Lithium-ion batteries, particularly focusing on improvements to energy density.

Introduction to KTP

A KTP (Knowledge Transfer Partnership) is a collaboration between a university and a company, jointly funded by the Company and Innovate UK. KTPs aim to help businesses improve their competitiveness and productivity through the better use of knowledge, technology and skills that reside within the UK Knowledge Base. This KTP is a 24-month project between Loughborough University and Echion Technologies Limited.

Introduction to the company

Echion Technologies Ltd. is a materials research and development business and world-leading developer of advanced lithium-ion battery materials. Echion products enable cell manufacturers to deliver cost-effective, fast-charging, high-energy density and long-life power cells for a wide range of markets including automotive, premium consumer electronics, and grid-storage applications. The company provides materials and battery cell manufacturers with packages of protected intellectual property, customisation options, materials synthesis and cell integration know-how for a variety of end-user markets.

Echion has a portfolio of patents in the area of Mixed Niobium Oxide anode materials and is regarded as a deep-tech start-up success story. To date the company has worked on several successful innovative projects with partners such as Vantage Power, QinetiQ, University of Birmingham, University of Cambridge, UCL, and Johnson Matthey. The projects have focused on topics ranging from technical development to market assessment and joint commercialisation plans aiming to bring innovations to market. More recently Echion has successfully completed their £10M Series-A funding round, led by CBMM – the world's leading supplier of niobium products and BGF – the UK & Ireland's most active and dynamic investor of equity capital in growth economy companies, with Cambridge Enterprise, Origin Capital and other existing shareholders also taking part.

University/Department summary

Loughborough University is a top-5 UK university, consistently ranked by the Guardian and other league tables. Its position as a research-leading university is confirmed through outstanding research in science and engineering and world-class research facilities. It has been awarded a record of seven Queen's Anniversary prizes for its research impact to society and UK industry.

With an international reputation for research excellence and track record in high quality training the Department of Chemistry at Loughborough University comprises 26 research active academic staff members, as well as more than 20 visiting/Emeritus academics, technical and support staff. The department is located on the Loughborough University campus, housing world-class research facilities. This new home for Chemistry opened in April 2018 following over £17M investment in infrastructure and the project is underpinned by substantial investment in High Performance Computing. LU is a partner of EPSRC National Tier 2 computational facility (HPC Midlands+, £3M) and a recently upgraded local HPC cluster (LoveLace, £1.12M), forming a sound basis for the advanced modelling required. As a founding member of a consortium of the Midlands' 6 research intensive universities the University collaboratively creates links sharing its resources with other leading researchers in order to deliver world-class research and innovations across the discipline and greater economic benefit.

The Loughborough University research team are experts in a range of computational methods including quantum mechanical packages extending to long time scale molecular dynamical simulations.

Project Outline

The technical goal of the KTP is to improve understanding of active anode materials stability in response to various modifications in order to improve energy density, ultimately providing in silico modelling to support R&D. The materials of focus will be proprietary Mixed Niobium Oxide structures that provide the ability to reversibly fast-charge/discharge a lithium-ion cell with significant advantages over current in market solutions. This will be delivered initially through enhanced understanding of crystal-level modifications, introduction of defects, potentially expanding the scope to grain boundary considerations.

Through an experimental approach Echion has developed a range of crystal structures and compositions that demonstrate affordable market-leading fast-charge performance (full charge in <5 mins) without sacrificing energy density or lifetime. A number of important areas can now be addressed using materials-modelling approaches.

Using Loughborough University's existing knowledge-base and expertise in materials-based modelling and academic research facilities the successful candidate will work with Echion to combine the approach with the companies pre-existing cell modelling work generating holistic, differentiated solutions.

The project will be delivered through the following objectives:

- Thermodynamic materials modelling
- Electronic/ionic modelling for product variations
- Combining modelling with experimentation to improve energy density
- Deployment of expertise into licensing / non-recurring engineering (NRE) packages

The successful Associate will be based within Echion Technologies Ltd. team in Cambridge, but will work closely with academics at Loughborough University, Loughborough campus.

Joint fortnightly research meetings and monthly KTP management meetings will be supported by the Echion team as well as Loughborough University researchers. The project will involve project management, organisational skills and strong communication skills. A travel budget of £1,000 is allocated for travel between Cambridge and Loughborough, as well as to other sites/clients as appropriate. There is also a training and development budget allocated to the project and it is expected that the associate will spend 10% of their time on personal and career development. The successful applicant will also receive a £2,000 per annum training budget.

We actively encourage applicants from women, LGBTQ+, disabled and Black, Asian and Minority Ethnic candidates, who will positively bring their experiences and voices to the partnership.

Job Description and Person Specification

Job Grade: Other

Job Purpose

The KTP Associate will:

- Apply academic theory to improve active battery materials that are currently of commercial interest
- Develop prototype models based on collated requirements for the product
- Developing realistic models of the active materials and variations thereof
- Answer research questions whilst describing method limitations to aid experimental design success
- Undertake necessary training for personal and career development
- Transfer the knowledge gained from compositional models to real life experimental work to improve electrochemistry performance
- Produce reports to senior management team
- Provide training materials/workshops to Echion staff as necessary
- Mentoring junior colleagues
- Produce marketing materials and technical online content to inform key business partners
- Contribute to academic research papers and intellectual property capture

Job Duties

- Carry out the KTP project tasks within a cutting-edge area of materials modelling and deliver the outcomes as outlined in the project plan
- Manage the project, applying materials modelling to an exciting and demanding business environment and disseminate the findings to the project team
- Undertake KTP management training, as well as other courses as deemed necessary
- Write R&D reports and presentations sharing these as project updates at the Local Management Committee (LMC) meetings, at national conferences and symposia and with the Echion Technologies team
- Update the Echion Technologies business development team with research outputs and developments for commercialisation of findings. Generate invention disclosure forms and assist the capture of intellectual property through pre-patent writing pre-patent technical invention reports.
- Travel to Company business partners within the UK, as required
- To undertake other such duties as may be reasonably requested and that are commensurate with the nature and grade of the post

Points to Note

The purpose of this job description is to indicate the general level of duties and responsibility of the post. The detailed duties may vary from time to time without changing the general character or level of responsibility entailed.

Previous KTP Associates or employees of Echion Technologies are not normally eligible to apply for this KTP

Applicants must have completed their last qualification (degree, masters, PhD) no more than five years before closing date.

Special Conditions

All staff have a statutory responsibility to take reasonable care of themselves, others and the environment and to prevent harm by their acts or omissions. All staff are therefore required to adhere to the University's Health, Safety and Environmental Policy & Procedures.

All staff should hold a duty and commitment to observing the University's Equality & Diversity policy and procedures at all times. Duties must be carried out in accordance with relevant Equality & Diversity legislation and University policies/procedures.

Successful completion of probation will be dependent on attendance at the University's mandatory courses which include Respecting Diversity and, where appropriate, Recruitment and Selection.

Organisational Responsibility

Reports to the KTP Lead Academic: Dr Pooja Goddard

Echion Lead Supervisor: Dr Alex Groombridge

Person Specification

Your application will be reviewed against the essential and desirable criteria listed below. Applicants are strongly advised to explicitly state and evidence how they meet each of the essential (and desirable) criteria in their application. Stages of assessment are as follows:

- 1 – Application
- 2 – Presentation
- 3 – Interview

Essential Criteria

Area	Criteria	Stage
Experience	Working experience of developing and fitting potential models with a record of accomplishment that includes dynamical studies of bulk as well as surfaces.	1,2,3
	Extensive DFT experience and/or possibly long timescale dynamics.	1,3
	Experience of presenting scientific data, reports, publications and presentations.	1,2,3
Skills and abilities	Proficient in managing large and complicated data sets and have good Python programming skills	1,3
	Excellent presentation / communication skills including the ability to write project reports and make technical presentations to industrial and academic research groups	1,2,3
	Ability to work both independently, without supervision, and, as part of a team	1,3
	Ability to deliver to tight deadlines and work in a flexible, methodical and conscientious approach	1,3
	Ability to communicate with a wide range of academic and commercial personnel	1,2,3
Training	Willingness to undertake KTP training modules and other training as appropriate	3
Qualifications	PhD in a relevant field such as Chemistry, Physics, Materials or Applied Mathematics.	1,3
Other	To observe the University Equal Opportunities policies at all times	3

Desirable Criteria

Area	Criteria	Stage
Functional/Technical	Knowledge of battery materials and how batteries work	1,3
Experience	Experience working in R&D projects	1,3
	Experience in project management	1,3
Skills and abilities	Excellent written and oral communication skills	1,3
	Excellent interpersonal, and organisational skills	1,3
	Ability to take part in collaborative activities and work with technical staff and people in other subject domains	1,3
	Strong real-world problem-solving skills	1,3
	Licensed to drive in the UK	1,3

Conditions of Service

The position is FULL TIME and FIXED TERM for 24 months. Salary will be between £30,000 - £40,000 per annum at a starting salary to be confirmed on offer of appointment. The successful applicant will also receive a £2,000 per annum training budget.

The appointment will be subject to the University's normal Terms and Conditions of Employment for Academic and Related staff/Operational and Administrative staff, details of which can be found [here](#).

We strive to create a culture that supports equality and celebrates diversity throughout the campus. The University holds a Bronze Athena SWAN award which recognises the importance of support for women at all stages of their academic career. For further information on Athena SWAN see <http://www.lboro.ac.uk/services/hr/athena-swan/>.

Applications

This is a re-advertisement and previous applicants need not apply.

The closing date for receipt of applications Wednesday 1 December 2021

The interviews will take place on Thursday 18th and Friday 19th November 2021. Please note that candidates may be invited for interview on any of these dates.