

Research Associate (fixed-term for 12 months)

Job Ref: REQ17674

As part of the University's ongoing commitment to redeployment, please note that this vacancy may be withdrawn at any stage of the recruitment process if a suitable redeployee is identified.

Job Description

Job Grade: Specialist and Supporting Academic Grade 6

Job Purpose

You will contribute to an INNOVATE-UK funded project on PROLAB: Practical and RObust Lithium Air Batteries. Working with Dr Pooja Panchmatia in the Advanced Materials Modelling group, you will contribute to a project involving the modelling and simulation of battery materials.

This position is part of a close collaboration between the Panchmatia group, University of Liverpool and Johnson Matthey (Reading, UK). Specifically, the job requires expert knowledge in atomistic interatomic based computational methods and Density Functional Theory (DFT). The project will also need some knowledge of battery materials, surface calculations and experience in any or all of these areas would be beneficial.

The successful candidate will also be expected to contribute to the formulation and submission of research publications and research proposals as well as help manage and direct this complex and challenging project as opportunities allow.

Job Duties

Research

- Design, model, and investigate bulk solid electrode/electrolyte materials to include defect chemistry and conduction.
- Develop/refine interatomic potentials and use DFT to investigate electrochemical properties of both the bulk and at surfaces.
- Identify surfaces and favourable morphologies and elucidate diffusion mechanisms at these surfaces.
- Liaise with experimental partners to design and enact interfacial interactions and model these using state
 of the art computational methods.
- Conduct independent and collaborative research in the development of interfacial models for energy storage devices.
- Work as part of a team, whilst delivering independent and self-directed activity.
- Work as part of the project team to assist in the writing of project reports, research papers, conference
 presentations and operational protocols.
- Build rapport with and act as a conduit to project partners across the UK.
- Monitor proficiency testing and statistical-processing and lead close collaboration with experimental and other modelling groups in the consortium.
- Engage with the wider Supergen and energy storage communities

Other activities

- Complete an agreed programme of professional development.
- Assist in the management and operation of the research systems in which this project is based.
- Engage in training programmes in the University (e.g. through Staff Development) which are consistent with your needs and aspirations and those of Chemistry.
- Undertake such other 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.

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.

The post holder may be required to work outside of normal office hours if necessitated by the exigencies of the service.

Organisational Responsibility

Reports to Principal Investigator, Dr. Pooja Panchmatia.

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 Test/Assessment Centre/Presentation
- 3 Interview

Essential Criteria

Area	Criteria	Stage
Qualifications	Relevant PhD in a relevant Chemistry/Physics/Materials field.	1
Experience	Developing/fitting interatomic potential models with a record of accomplishment that includes dynamical studies both in the bulk and/or surfaces.	1,2,3
	Management of large and complicated data sets.	1,3
	Preparation of scientific data, reports, papers and communications.	1,3
	Working to fixed deadlines.	1,3
Skills and Abilities	Excellent IT skills.	1
	A record of delivered presentations to a range of different audiences including industry and scientific conferences.	1,3
	Flexible, methodical and conscientious approach to work.	3
	Ability to work both independently and as a team member	1,3
Training	Demonstrate evidence of having undertaken further training .	1
Other	Evidence a good working knowledge of equal opportunities and understanding of diversity in the workplace	1,3

Desirable Criteria

Area	Criteria	Stage
Experience	Interface modelling.	1,3
Skills and Abilities	Experience of running independent project work.	1,3

Conditions of Service

The position is full time and fixed term for 12 months. Salary will be on Specialist and Supporting Academic Grade 6 (£29,301 - £38,183 per annum) at a starting salary to be confirmed on offer of appointment.

The appointment will be subject to the University's normal Terms and Conditions of Employment for Academic and Related staff, details of which can be found <u>here</u>.

The University is committed to enabling staff to maintain a healthy work-home balance and has a number of family-friendly policies which are available at http://www.lboro.ac.uk/services/hr/a-z/family-leave-policy-and-procedure---page.html.

We also offer an on-campus nursery with subsidised places, subsidised places at local holiday clubs and a childcare voucher scheme (further details are available at: <u>http://www.lboro.ac.uk/services/hr/a-z/childcare-information---page.html</u>

In addition, the University is supportive, wherever possible, of flexible working arrangements. We also 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. We encourage women to apply for this position as they are under-represented. All appointments will be made on merit. For further information on Athena SWAN see http://www.lboro.ac.uk/services/hr/athena-swan/

Informal Enquiries

Informal enquiries should be made to Dr. Pooja Panchmatia by email at: <u>p.panchmatia@lboro.ac.uk</u> or by telephone on +44 (0)1509 222548.