

Research Associate in Computational Modelling of Biomaterial Dissolution

REQ200472

As part of the University's ongoing commitment to redeployment, please note that this vacancy may be withdrawn at any stage of the recruitment process if a suitable redeployee is identified.

Project Description

Applications are invited for a Research Associate position at the Department of Materials, Loughborough University. This position is funded by the Leverhulme Trust, as part of a project entitled "Understanding biomaterial dissolution from computational modelling" and led by Dr Jamieson Christie. The successful applicant will join a group conducting novel and exciting research in computational design of biomaterials, with collaborations across the UK and overseas. Loughborough University has active research communities in biomaterials and in computational materials science, and is the location of the 14,336-core HPC Midlands Plus facility.

This position is well-suited to an ambitious early-career researcher with a background in computational materials science and a desire to pursue multidisciplinary research.

In this project, computational models of phosphate glasses will be constructed and the interactions of the glass with the body environment characterised, to understand how they can be optimised for specific applications. Phosphate glasses dissolve after implantation in the body at a rate which can be changed by several orders of magnitude, depending on composition. They can also incorporate therapeutic substances (e.g. drugs, antimicrobials) which makes them suitable for use as a mechanism for targeted delivery of a substance at a therapeutically appropriate rate.

The interaction of the material with the surrounding physiological environment is still poorly understood, and this project will focus on developing computational models that allow us to characterise the behaviour of the interface between the glass and the body, and so understand how the dissolution can be controlled and optimised for specific therapies. Previous work (see, e.g., *J. Mater. Chem. B* **5**, 5297 (2017)) has focussed mainly on the glass structure alone.

Job Description

Job Grade: Specialist and Supporting Academic Grade 6

Job Purpose

The postholder will conduct classical and first-principles molecular dynamics simulations of various compositions of phosphate glasses in the physiological environment. This will include the construction of accurate interatomic potentials to model the interaction between the glass and the surrounding aqueous environment. The aim will be to predict and explain the atomic mechanisms which control the dissolution of the glass and how they can be

controlled to optimise the use of the glass for specific therapeutic applications. The postholder will also disseminate this work through publications and attendance at conferences.

Job Duties

- To conduct computational simulations of phosphate glass compositions in the physiological environment.
- To construct accurate classical interatomic potentials for the simulation of phosphate glass compositions in the physiological environment.
- To compare the results of these simulations to other experimental and computational data, and understand the factors which affect the dissolution rate of phosphate glasses when implanted into the body.
- To use the results obtained to predict strategies for optimising the use of phosphate glass as an implanted biomaterial for specific therapeutic applications.
- To be responsible for conducting the day-to-day running of the project.
- To write research papers suitable for publication in high-quality academic journals.
- To present research work at relevant academic conferences.
- To prepare, or assist in the preparation of, applications for time on HPC resources.
- To assist with the supervision of PhD, MSc and undergraduate project work in related areas.
- To engage in training programmes in the University (or elsewhere) that are consistent with the needs of the project and the Department.
- To undertake 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.

The postholder would be welcome to involve themselves in the University's teaching activities, where appropriate.

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 Dr Jamieson Christie, Senior Lecturer, Department of Materials.

Person Specification

Your application will be reviewed with respect to meeting the essential and desirable criteria listed below. 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
Experience	Experience in molecular dynamics simulations of materials	1, 3
	Experience in the use of high-performance computing facilities	1, 3
	Experience in writing research papers suitable for publication in high-quality journals	1, 3
	Experience in project planning and management	1, 3
Skills and abilities	Knowledge of appropriate computational methods for the simulation of materials in various environments	1, 3
	Excellent oral and written presentation skills	1, 3
	Able to coordinate project tasks, manage project work, prioritise competing tasks, and meet deadlines	1, 3
	Able to work both independently and as part of a team	1, 3
	Have a working knowledge of computing environments for data analysis and post-processing, such as Matlab and Python	1, 3
	Able to strengthen the group's existing collaborations, and establish new collaborations	1, 3
Training	Willing to undertake further training as appropriate and to adopt new procedures as required	1, 3
Qualifications	A PhD (or one close to completion) in materials science, chemistry, physics, or a related discipline	1, 3
Other	A commitment to following the University's Equality and Diversity policies at all times	1, 3

Desirable Criteria

Area	Criteria	Stage
Experience	Experience in the supervision of other postgraduate or undergraduate students	1, 3
	Experience in teaching scientific or engineering topics at postgraduate or undergraduate level	1, 3
	Experience in the development of interatomic force fields (potentials)	1, 3
	Experience in research into amorphous materials and/or glasses	1, 3

Conditions of Service

The position is **full-time** and **fixed-term** for 33 months. The successful candidate is expected to commence their role on 1 October 2020 or as soon as possible thereafter. Salary will be on Specialist and Supporting Academic Research Grade 6, (£30,942 - £40,322 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 Grade 6 and above staff, details of which can be found [here](#).

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: <http://www.lboro.ac.uk/services/hr/a-z/childcare-information---page.html>).

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. For further information on Athena SWAN see <http://www.lboro.ac.uk/services/hr/athena-swan/>.