

Research Associate in Interatomic Potential Development for Simulation of Bulk Metallic Glasses (Part or Full time)

Job Ref: REQ240068

As part of the University's ongoing commitment to redeployment, please note that this vacancy may be withdrawn at any stage of the recruitment process if a suitable redeployee is identified.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

Molecular dynamics (MD) simulations are an effective way of understanding the connections between a material's composition, and its structure and properties. For these simulations to be accurate, the interatomic forces must be well represented with an accurate expression for the potential energy (the 'potential'). In this project, the researcher will develop and use accurate potentials for the simulation of bulk metallic glass (BMG).

BMGs show potential as biomaterials due to properties such as low Young's modulus, high fracture strength and excellent corrosion resistance. This project forms part of ongoing computational and experimental work to understand how to optimise the suitability of BMGs for orthopaedic applications. For many interesting BMG compositions, existing potentials are inaccurate, and the central task of the project is to develop improved potentials and validate them in simulation by comparison to experimental data.

We are willing to consider filling the post at lower FTE, e.g., part-time, to allow, for example, the researcher to complete another piece of work, such as writing up their PhD, or to fulfil caring or other personal responsibilities.

Job Description

Job Grade: Specialist and Supporting Academic Grade 6

Job Purpose

To conduct research in computer simulation of BMGs using molecular dynamics. Specifically, to develop new potentials which accurately represent the interatomic forces in BMGs and to validate them both in simulation and against experimental data. To use these insights to understand the connections between BMG composition, structure and properties. To generate scientific results suitable for publication in high-quality journals. To collaborate with other members of the team.

Job Duties

- To parametrise interatomic potentials suitable for biomedically relevant bulk metallic glass compositions, and use those potentials in classical molecular dynamics simulations of different BMGs.
- To use simulations, combined with experimental data taken in the group, to understand how the composition and structure of the glass affects its properties, including its suitability for biomedical applications.
- To conduct research of academic rigour and high scientific standard, of a level suitable for publishing in high-quality journals, consistent with the Schools' and Research Lab's quality and ambition.
- To assist the academic staff in the project team with the supervision of undergraduate, MSc and PhD project work and day-to-day supervision and support of other researchers.

- To keep all other investigators and collaborators, including those located at other institutions, regularly apprised of the progress of the work, including recommendations for next steps.
- To work as part of a multi-disciplinary, multi-location team that addresses different aspects of metallic glass properties.
- Travel to external partners and collaborators, attend meetings and make presentations, when required.
- To attend and contribute to conferences, seminars, webinars and other events of interest to the team.
- To contribute to project promotion and public engagement events.
- To contribute ideas for new research and impact directions.
- To maintain confidentiality and ensure that intellectual property (IPR) generation is safeguarded, and agreements are not violated.
- To engage in training programmes in the University (or elsewhere) that are consistent with the needs and aspirations of the project and those of the Lab.
- 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. Training will be provided as necessary and in support of the Researchers' professional development, and an attitude for learning will be an essential criterion in the selection of a successful candidate.

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 Prof Carmen Torres-Sanchez, Principal Investigator, and Dr Jamieson Christie, Department of Materials, co-investigator.

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/Presentation
- 3 – Interview

Essential Criteria

Area	Criteria	Stage
Experience	Experience in the parametrisation of interatomic potentials for classical molecular dynamics simulations	1,2,3
	Experience in using classical molecular dynamics simulations to understand the connections between the structure and property of materials	1,2,3
	Conducting research of academic rigour and high scientific standard	1,2,3
	Authoring manuscripts and high-quality journal papers for publication	1
	Basic understanding of bulk metallic glasses	1,2,3
	Practical modelling, optimisation and visualisation skills with software, relevant to amorphous alloys	1,2,3
	Experience presenting to a variety of audiences, from technical and expert to general practitioners	1,2,3
Skills and abilities	Ability to work accurately and precisely and to record information gathered	2, 3
	Self-motivated and able to work without close supervision, especially when working remotely	3
	Ability to work to deadlines	1,3
	Ability to work independently and as part of a team	1,3
	Ability to maintain confidentiality	3
	Ability to work accurately and precisely and to record information gathered	1,2,3
Qualifications	Ph.D. completed (or about to complete) in Materials Science, Physics, Mathematics, Computer Science or Engineering	1,3
	Good First Degree in Materials Science, Physics, Mathematics, Computer Science or Engineering (1 st or 2.1 equivalent)	1

Desirable Criteria

Area	Criteria	Stage
Experience	Knowledge and deep understanding of bulk metallic glasses, especially those relevant biomedically	1,2,3
	Able to work in multi-disciplinary teams	1,3
Skills and abilities	Experience working at the simulation/experimentation interface	1,2,3
Qualifications	Ethical and risk assessment trained	1,3
Other	Able to travel within the UK	1,3

Conditions of Service

The position is FIXED TERM for 6 MONTHS with the possibility of an extension based on performance and initial results. Salary will be on Specialist and Supporting Academic Grade 6, £33,966 - £44,263 per annum, depending on the candidate's experience at the time of appointment.

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](#).

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/>