

## Research Associate

### *Modelling Reduced Activation High Entropy Alloys*

Job Ref: REQ190547

**As part of the University's ongoing commitment to redeployment, please note that this vacancy may be withdrawn at any stage of the recruitment process if a suitable redeployee is identified.**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

The work involves modelling multicomponent alloys with the key tasks described below.

## Job Description

**Job Grade:** Specialist and Supporting Academic Grade 6

The work will involve conducting research into multicomponent High Entropy Alloys, to determine their mechanical and thermal properties from first principles. Furthermore, by using multiscale modelling techniques, the work will involve assessing the radiation resistance of various candidate alloys. The project will require use of Loughborough's high-performance computing system and will entail developing and running software on the system.

## Job Duties

- To model the mechanical and thermal properties of various multicomponent high entropy alloys from first principles.
- To investigate the applicability of the various models.
- To carry out modelling of radiation effects in high entropy alloys using molecular dynamics (MD) and long-time scale methods.
- To discuss the results and their interpretation, as appropriate.
- To interact effectively with the experimental collaborators in the project.
- To disseminate non-confidential results both at conferences and in the scientific literature.
- To liaise with staff members, help with supervising research students and to ensure objectives and milestones within the project are met.
- To undertake tasks assigned by the principle and co-Investigators.
- To model the mechanical and thermal properties of various multicomponent alloys from first principles.
- To investigate defects in the materials.
- To develop multiscale modelling tools so that larger systems can be studied.
- To analyse the damage produced by the primary radiation in the materials.
- To liaise with experimental collaborators on an associated EPSRC programme.
- Be responsible for conducting the day to day running of the project.
- To formulate detailed plans for the project based on broad guidance from the project team.
- To feed back to the project team on progress, to make recommendations for next steps.
- Write up regular progress reports and present outcomes to all Investigators and Collaborators.
- Travel to attend meetings and make presentations both within the project partners working group and to external stakeholders.
- To support the project team by enhancing relationships with existing collaborators and by assisting the establishment of relationships with new collaborators.

- To write research papers suitable for publication in high quality academic journals.
- To attend and contribute to conferences.
- To contribute to project promotion and public engagement events.
- Contribute ideas for new research and enterprise directions.
- Maintain confidentiality at all times and ensure that intellectual property (IPR) agreements are not violated.
- 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.
- Where appropriate, to deliver teaching, tutorial and laboratory sessions to students.
- Engage in training programmes in the University (or elsewhere) that are consistent with the needs and aspirations of the project and those of the Department.
- 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.

### **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 Principle and Co-Investigators.

## 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
Experience	Experience of conducting research in modelling within materials science	1,3
	Experience of publishing research outcomes	1,3
	Experience with, Density Functional Theory, Molecular Dynamics and Monte-Carlo models	1,3
Skills and abilities	Ability to publish in international journals	1,3
	Excellent oral communication skills to present material at International meetings	3
	Strong analytical mathematical skills Competence of programming in C, FORTRAN, Python or a similar language	1,3
	Ability to work as part of a team and to collaborate with others.	3
	Self-motivated with ability to meet deadlines	1,3
	Excellent interpersonal, and organisational skills	1,3
	Ability to write project reports and make technical presentations to industrial and academic research groups	1,3
	Knowledge of relevant Health & Safety issues	1,3
Training	A willingness to undertake further training as appropriate and to adopt new procedures as and when required	3
Qualifications	Post Graduate qualification in the Physical Sciences, Mathematics, Computing or Materials	1,3
Other	Commitment to observing the University's Equal Opportunities policy at all times	3

### Desirable Criteria

Area	Criteria	Stage
Experience	Experience of modelling radiation effects	1,3
	Experience with long time scale atomistic methods and EAM/MEAM potentials	1,3
	Developing proposals for funding from external agencies	1,3
Skills and abilities	Competence in high performance computing and scripting languages	1,3
	Competence in parallel programming	3
	Experience with CALPHAD or similar methods for investigating material phases	1,3
	Experience of linking theoretical models with experiments	3
	Some understanding of the SQS method and the ATAT software	1,3
	A strong publication track record	1,3

Other	Ability to travel to attend meetings	1,3
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## Conditions of Service

The position is full time and fixed term for up to a maximum 36 months, not extending beyond 14/10/22. Salary will be on Specialist and Support Academic, Grade 6 (£30,395 - £35,211) per annum, at a starting salary to be confirmed on offer of appointment.

The appointment will be subject to the University's Terms and Conditions of Employment for Staff Grades 6 and above 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 can be found [here](#).

The University offers a wide range of employee benefits which can be found [here](#).

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/>

## Applications

The closing date for receipt of applications is **18 August 2019**.