

## Research Associate in Computational Chemistry

### *Atomistic Modelling of High Energy Materials*

### Fixed Term for 12 Months

Job Ref: REQ231362

#### Project Description

Applications are invited for a postdoctoral research associate position in computational chemistry. This is a DSTL funded position to work with Dr Kenny Jolley and Dr Felix Plasser (Chemistry, Loughborough University) on predicting the crystal structure, dynamics and physical properties of energetic materials.

Predicting the crystal structure of complex mixtures of energetic compounds is a difficult task. The direct approach of simulated annealing using molecular dynamics is not feasible because it requires simulation time scales of hours/days. Therefore, the successful applicant will use time accelerated methods including temperature accelerated MD, adaptive on-the-fly kinetic Monte-Carlo, and parallel replica 'ParSplice' methods. Alternative optimisation techniques to predict crystal structures will also be investigated including, particle swarm optimization, the CALYPSO code, and machine learning methods.

The successful applicant will also conduct molecular dynamics (MD) simulations on the bulk crystal structures of complex mixtures of energetic compounds, to investigate their properties. Bulk physical properties, stability to shock and heat, and reaction pathways will be modelled and compared to experimental data. This will require modelling complex initial conditions including thermal spikes, and shockwaves. Analysis of reaction pathways and compositions of products will be required.

Applicants should hold (or be about to obtain) a PhD in a relevant field (e. g., Physics, Chemistry, Materials Science or Applied Mathematics). Experience of computational modelling using molecular dynamics (particularly using LAMMPS on high performance computing clusters) and kinetic Monte-Carlo (kMC) is desired. Computer programming skills (C/C++ or FORTRAN) and data analysis skills using Python are desired.

This position is ideally suited for an ambitious early career researcher with a background in computational chemistry and materials modelling. The successful candidate will be highly motivated with a strong research track record and a desire to pursue multidisciplinary research.

#### Job Description

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

**Job Purpose:** This is a DSTL funded position to develop theoretical computational models to predict the crystal structure and physical properties of energetic materials.

#### Job Duties

#### RESEARCH AND SCHOLARSHIP

- Develop the techniques for predicting the crystal structures of energetic chemical compounds and mixtures thereof.
- Design complex MD simulations to investigate the physical properties of these materials including their stability to shock and heat.
- Analyse the data obtained and discuss the interpretation of the results.
- Prepare and deliver project updates to DSTL.
- Lead the preparation of research articles for submission to high-quality chemistry journals.
- To contribute to project promotion and public engagement events including conferences.
- Continually update knowledge and understanding in the field and translate advances into research activity.
- Plan and manage research activities in collaboration with others, with guidance if required.
- Communicate research material at conferences and at meetings with collaborators.
- Build external contacts and participate in the exchange of knowledge at conferences/networks to form relationships for future collaboration.
- Assist with the preparation of proposals and applications for funding to external bodies.
- Interact effectively with collaborators during the project.

## **TEACHING AND LEARNING**

- Assist in the supervision and management of undergraduate (MChem/MSc) research projects.
- Where appropriate, deliver teaching and tutorial sessions to undergraduate students.
- May assist in the development of student research skills.
- Engage in training programmes in the University (e.g. through staff development), which are consistent with your needs and aspirations and those of Chemistry.

## **OTHER ACTIVITIES**

- Assist with the management and smooth operation of equipment within the research group.
- Undertake other duties that may be reasonably requested and 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 is subject to DSTL security clearances.

## **Organisational Responsibility**

Reports to Dr Kenny Jolley, Lecturer in Chemistry.

## 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	Holds (or is about to obtain) a PhD in a relevant field (i.e., Physics, Chemistry or Applied Mathematics).	1
Experience and Knowledge	Experience of performing atomistic computer simulations of materials or molecules.	1
	Research experience with sufficient depth of specialist knowledge in chemistry.	1,3
	Preparation of scientific reports and research publications.	1,3
	Advanced knowledge of the research methods and techniques to work effectively within the research programme.	1,3
	Will continually update knowledge in the field and engage in continuous professional development.	3
Skills and Abilities	Excellent written and oral communication skills.	1,3
	Ability to organise time, plan research and work independently.	1
	Ability to work in a team and strong interpersonal skills.	1
	Ability to deliver oral presentations, write internal research reports and produce draft publications.	1,3
	Self-motivation and ability to meet fixed deadlines.	1,3
Training	Ability to share responsibility for the supervision and training of post-graduate and undergraduate research students.	1,3

### Desirable Criteria

Area	Criteria	Stage
Experience and Knowledge	Experience of performing computational simulations using molecular dynamics using LAMMPS on high performance computing clusters.	1,3
	Experience of long time-scale computational modelling techniques.	1,3
	Competence in high performance computing and scripting languages such as Python.	1,3
	Competence in parallel programming.	1,3
	Experience in designing complex simulations for modelling shockwaves, thermal spikes, and cascade reactions.	1,3

## Conditions of Service

The position is full-time and fixed term for a period of 12 months. Salary will be on research grade 6 (£33,966 – £44,263 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 [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/>

## Informal Enquiries

Informal enquiries should be made to Dr Kenny Jolley by email at [k.jolley@lboro.ac.uk](mailto:k.jolley@lboro.ac.uk).

## Applications

The closing date for receipt of applications is 24/11/2023.