

RESEARCH ASSOCIATE IN COMPUTATIONAL CHEMISTRY AND MACHINE LEARNING

Job Ref: REQ260237

School/Department summary

Loughborough University is seeking to appoint a Postdoctoral Research Associate in the area of Computational Chemistry and Machine Learning to conduct research under the direction of Dr Felix Plasser on a DSTL funded project “Computational Analysis of High Energy Materials” with the aim of developing and applying computational methods to predict the detonation parameters of energetic materials.

Applicants should hold (or be about to obtain) a PhD in a relevant field (e.g., Computer Science, Chemistry, or Physics). Computer programming skills (python) are essential. Practical experience in developing machine learning models is desired. The appointee will be based in the Department of Chemistry at Loughborough University.

Job Description

Job Family and Grade: Specialist and Supporting Academic Grade 6

Job Purpose

To conduct research under the direction of Dr Felix Plasser on a DSTL funded project “Computational Analysis of High Energy Materials”. The applicant will become part of Dr Plasser’s research team in Computational Chemistry.

Job Duties

To conduct research on the project described above. This will involve a combination of individual work and collaborative work.

- Development of inverse design protocols for energetic materials based on our existing machine learning framework (*J. Chem. Theory Comput.* 2025, 21, 17, 8406–8419).
- Rewriting the above machine learning framework for enhanced portability and performance.
- Interpretation of machine learning results to explain which molecular features are most influential in energetic materials design.
- To become familiar and critically assess the relevant literature on computational high-energy materials
- To meet regularly with the PI, to discuss the progress of the project, and to report the findings of research undertaken to the PI and DSTL representatives.
- To prepare journal publications of results arising from the project.
- To take part in relevant research related activities within the Department of Chemistry. This may include both taking part and delivering research seminars, and to participate in relevant Working Groups that may be set up during the course of the project.
- To be an active member of the PI’s research group attending and contributing to research seminars as well as providing guidance to other group members.
- To attend and contribute to conferences.
- 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.

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 outlined in the document.

The post is subject to DSTL security clearances.

Organisational Responsibility

Reports to: Dr Felix Plasser, Senior Lecturer in Physical Chemistry

Direct Reports: N/A

Budget Responsibilities: N/A

Structure Chart: N/A

Person Specification

Your application will be assessed based on the essential and desirable criteria listed below.

Applicants are strongly encouraged to explicitly demonstrate how they meet each essential (and desirable) criteria at the application stage. The criteria that you need to demonstrate in your application will be listed as Stage 1 in the table below.

Stages of assessment are as follows:

- 1 – Criteria measured within the Application
- 2 – Criteria measured at Test/Assessment Centre/Presentation
- 3 - Criteria measured at Interview

Essential Criteria: When completing the section below, clearly state the essential requirements of the role and think broadly. Focus on what must be accomplished rather than how it should be done. Consider experience outside of higher education where appropriate. Avoid requiring all criteria to be measurable from the application form; for example, skills and abilities may be better assessed through tests/ assessments and/ or interviews. As a rule, aim for no more than 5-7 criteria to be measured at the application stage.

Area	Criteria	Stage
Experience	Experience of conducting research in machine learning	1,3
	Published papers on machine learning	1
Skills and abilities	Ability to carry out high-level rigorous research	1,3
	Excellent computer programming and general IT skills	1,3
	Excellent written and oral communication skills	1,3
	Self-motivated with ability to meet deadlines	1,3
	Able to manage time and task effectively to meet project deadlines and prioritise workload with minimum supervision	1,3
	Able to build and maintain effective working relationships with academic colleagues, students, and external partners to support collaborative research and communication of findings	1,3
	Knowledge of relevant Health & Safety issues	1,3
Qualifications	PhD (or near completion)	1
Other	Uphold and actively contribute to the University's commitment to Equity, Diversity and Inclusion.	1,3

Desirable Criteria: These are skills, experience and competencies that are additional extras that may be used to narrow the pool down if we receive a high volume of applications that meet the essential criteria.

Area	Criteria	Stage
Experience	Practical experience of developing machine learning models using python	1
Skills and abilities	A strong publication track record (career appropriate)	1
	Detailed understanding of advanced machine learning aspects (feature selection, operation of neural networks)	1,3

Conditions of Service

The appointment will be subject to the [University's Terms and Conditions of Employment](#) relevant to the job grade.

Shared University Responsibilities

As a member of the Loughborough community, you are expected to:

- Take reasonable care of yourself, others and the environment, and to prevent harm by your acts or omissions. All staff are therefore required to adhere to the University's Health, Safety and Environmental Sustainability Policies & Procedures.
- Support and contribute to the University's commitment to Equity, Diversity, and Inclusion (EDI), while carrying out all duties in a way that respects these principles and upholds the right to free expression. Further information about EDI at Loughborough and our strategic aims is available on our website.

Our Purpose, Vision, and Values

Our purpose, Vision and Values underpin all that we do and shape how we work together at Loughborough.

We're proud to promote our values: **Adventurous**, **Collaborative**, **Creative**, **Authentic** and **Responsible**. Our people bring these values to life every day, and they are central to the positive and supportive culture that makes Loughborough unique.

If you join us, you'll be encouraged to bring these values to life in your own work and contribute to the positive, supportive culture that makes Loughborough unique.

Read more about our [vision and values](#).

Our Accreditations



We strive to create a culture that supports equity 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 career.



We are proud to be a [Race Equality Charter Member](#). The Charter aims to improve the representation, progression and success of all minority ethnic staff and students within higher education and address issues of racism within higher education institutions (HEIs).



We are proud to be a Disability Confident Employer and have adopted a proactive approach to employing disabled people and to creating a more diverse workforce. We ensure that our recruitment processes are inclusive and accessible. We guarantee to offer an interview to all applicants who have declared a disability, provided that the essential criteria for the role are met. We proactively anticipate and provide reasonable adjustments and support existing employees who acquire a disability or long-term condition to thrive in the workplace.



We are a real living wage employer, and our Living Wage Employer Mark shows our commitment to paying our staff according to the cost of living.



We are proud supporters of the [City of Sanctuary movement](#) and delighted to be recognised as a University of Sanctuary. This national network brings together, university staff, lecturers, academics, and students, who together work to make Higher Education institutions places of safety, solidarity and empowerment for people seeking sanctuary.

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.