UNIVERSITY OF LEEDS

CANDIDATE BRIEF

Research Fellow in AI and Computational Chemistry, Faculty of Engineering and Physical Sciences

Salary: Grade 7 (£41,064 – £48,822 p.a.)

Reporting to: Dr Bao Nguyen

Reference: EPSCH1127

Closing date: Tuesday 17 February 2026

Fixed term (24 months - to complete specific time limited work)

Location: Leeds main campus (with scope for hybrid working)

We are open to discussing flexible working arrangements.

Research Fellow in AI and Computational Chemistry, School of Chemistry.

Are you interested in developing interpretable AI models for the next generation of green syntheses? Do you have experience in AI/Machine Learning, or computational modelling of organic reactions? Do you want to work in a high interdisciplinary at the heart of one of the UK's leading research-intensive universities?

Overview of the Role

The switch from traditional organic solvents, many of which are hazardous, volatile or non-sustainable, to modern green solvents is one of the key sustainability objectives in High Value Chemical Manufacture. Currently, the use of green solvents is often explored at process development stage, instead of discovery stage, leading to reoptimisation, longer development time, cost, and additional uncertainty. On the other hand, selecting the right solvent early may enhance chemoselectivity, avoid additional reaction steps, and simplify purification of the products.

Predicting these changes is an important underpinning capability for wider adaptation of green solvents in manufacturing, and there is an urgent need for ML models which predict reactivity in green solvents based on available data in traditional solvents. In this interdisciplinary project, you will develop solvent-dependent reactivity and reaction selectivity prediction models for green solvents, based on reactivity data curated from the literature and DFT/cheminformatics derived reactivity descriptors. You will also produce a standard set of substrates based on cheminformatics analysis of industrially relevant reactions for reaction scope, and limitations study by the synthetic community. These outputs will have transformative impacts in the chemical manufacture industry, delivering rapid, more sustainable and better quality-controlled processes through shorter development time, and confidence in predicting reaction outcomes in green solvents. The project will be carried out with support from industrial partners working in the field of cheminformatics and AI/Machine learning and end-users in High Value Chemical Manufacturing: Lhasa Ltd., Molecule One, AstraZeneca, CatSci, and Concept Life Science.

Working in a collaborative research team based in the Institute of Process Research & Development, you will lead the analysis of curated reaction data and will develop reactivity descriptors based on 2D and 3D structures (generated with high throughput DFT calculations) of organic substrates and reagents. You will develop a set of standard substrates based on analysis of industrial substrates and lead the development of solvent-dependent reactivity prediction models in green solvents.

Co-ordinating with collaborators at University of Southampton (data mining and curation) and Imperial College London (experimental data collection and validation) on these tasks; you will manage collaborations with industrial partners during the project and employ High Performance Computing, Python programming, DFT calculations and ML algorithms to deliver the objectives of the project.

Holding a PhD in Chemistry (or have submitted your thesis before taking up the role); you will have a strong background in Python programming and computational chemistry coupled with experience in working in an interdisciplinary team with industrial partners.

Main duties and responsibilities

- Develop a set of standard substrates for organic reactions relevant to industry;
- Carry out reaction data analysis and descriptor development for organic reactivity with cheminformatics and DFT calculations;
- Develop and rationally improve AI models for solvent dependent reactivity and generate selectivity predictions in green solvents for standard substrates, and validate them with experimental data from Imperial College London;
- Coordinate with other team members at University of Southampton and Imperial College London and technical partners at Lhasa Ltd, and Molecule One to achieve the project's objectives;
- Regularly presenting results to the industrial advisory board and collaborate with its members on translational activities;
- Generating and pursuing independent and original research ideas in the
- appropriate subject area;
- Developing research objectives and proposals and contributing to setting the direction of the research project and team including preparing proposals for
- funding in collaboration with colleagues;
- Evaluating methods and techniques used and results obtained by other

researchers and to relate such evaluations appropriately to your own research;
- Making a significant contribution to the dissemination of research results by publication in leading peer-reviewed journals and by presentation at national
- and international meetings;
- Working independently and as part of a larger team of researchers, both internally and externally, to develop new research links and collaborations and engage in knowledge transfer activities where appropriate;
- Maintaining your own continuing professional development and acting as a mentor to less experienced colleagues as appropriate;
- Contributing to the training of both undergraduate and postgraduate students, including assisting with the supervision of projects in areas relevant to the project.

These duties provide a framework for the role and should not be regarded as a definitive list. Other reasonable duties may be required consistent with the grade of the post.

Qualifications and skills

Essential

- A PhD in Chemistry (or have submitted your thesis before taking up the role) or a closely allied discipline;
- A strong background in data science and/or computational chemistry;
- Demonstratable experience in the following:
    - Cheminformatics;
    - Python programming;
    - Working in a collaboration with industrial partners;
- Good time management and planning skills, with the ability to meet tight deadlines and manage competing demands effectively without close support;
- A developing track record of peer reviewed publications in international journals;
- Excellent communication skills both written and verbal, and the ability to communicate your research at national and international conferences;
- A proven ability to work well both independently and in a team;
- A strong commitment to your own continuous professional development.

Desirable

- Experience of pursuing external funding to support research;
- Demonstratable experience in cheminformatics;
- Good knowledge of organic synthetic reactions;
- Demonstratable experience in green and sustainable chemistry.

How to apply

You can apply for this role online; more guidance can be found on our How to Apply information page. Applications should be submitted by **23:59** (UK time) on the advertised closing date.

Contact information

To explore the post further or for any queries you may have, please contact:

Dr Bao Nguyen, Associate Professor
Tel: +44 (0)113 343 0109
Email: B.Nguyen@leeds.ac.uk

Additional information

Faculty and School Information
Further information is available on the research and teaching activities of the Faculty of Engineering & Physical Sciences, and the School of Chemistry.

Working at Leeds
We are a campus-based community and regular interaction with campus is an expectation of all roles in line with academic and service needs and the requirements of the role. We are also open to discussing flexible working arrangements. To find out more about the benefits of working at the University and what it is like to live and work in the Leeds area visit our Working at Leeds information page.

A diverse workforce

As an international research-intensive university, we welcome students and staff from all walks of life and from across the world. We foster an inclusive environment where all can flourish and prosper, and we are proud of our strong commitment to student education. Within the Faculty of Engineering and Physical Sciences we are dedicated to diversifying our community and we welcome the unique contributions that individuals can bring, and particularly encourage applications from, but not limited to Black, Asian and ethnically diverse people; people who identify as LGBT+; and people with disabilities. Candidates will always be selected based on merit and ability.

The Faculty of Engineering and Physical Sciences are proud to have been awarded the Athena SWAN Silver Award from the Equality Challenge Unit, the national body that promotes equality in the higher education sector. Our equality and inclusion webpage provides more information.

Information for disabled candidates

Information for disabled candidates, impairments or health conditions, including requesting alternative formats, can be found under the 'Accessibility' heading on our How to Apply information page or by getting in touch by emailing HR via hr@leeds.ac.uk.

Criminal Record Information

Rehabilitation of Offenders Act 1974

A criminal record check is not required for this position. However, all applicants will be required to declare if they have any 'unspent' criminal offences, including those pending.

Any offer of appointment will be in accordance with our Criminal Records policy. You can find out more about required checks and declarations in our Criminal Records information page.

Salary Requirements of the Skilled Worker Visa Route

Please note that this post may be suitable for sponsorship under the Skilled Worker visa route but first-time applicants might need to qualify for salary concessions. For more information, please visit the Government's Skilled Worker visa page.

For research and academic posts, we will consider eligibility under the Global Talent visa. For more information, please visit [the Government's page, Apply for the Global Talent visa.]