CANDIDATE BRIEF
Research Fellow in Theoretical Calculations for Chemical Activation, Faculty of Engineering & Physical Sciences

Salary: Grade 7 (£33,797–£40,322 p.a.) Due to funding restrictions an appointment will not be made above £36,914 p.a.
Reference: EPSCH1044
Closing date: Friday 10 September 2021
Fixed-term until 31/05/2024
We will consider job share / flexible working arrangements
Research Fellow in Theoretical Calculations for Chemical Activation, School of Chemistry

Are you an experienced computational chemist looking to work in close conjunction with experimentalists to further our understanding of the molecular mechanisms of reactions? Are you looking to work with and develop an internationally recognised package, used by researchers from varying fields around the world?

The EPSRC has funded researchers at the Universities of Leeds and Oxford to examine the role of chemical activation in complex systems such as combustion and atmospheric chemistry. Chemical activation is where the reagents in a sequential reaction have retained some/all of the exothermicity of the reaction in which they were generated. Most models of complex systems assume thermalized distributions of reagents; chemical activation can accelerate processes and open up new channels in reactions.

The master equation programme MESMER has been developed and successfully deployed to model the temperature and pressure dependence of reactions. You will work closely with theoreticians and experimentalists to develop the MESMER code to better understand the fundamentals of chemical activation and how chemical activation can be included in practical models of complex systems such as combustion.

For a number of reactions in this project (carried out in both Leeds and Oxford), you will be able to use the current version of MESMER to model the experimental output for example probing the role of energy transfer, leading to thermalization, which will always be in competition with chemical activation. However, new or improved functionality will have to be developed within MESMER to account for chemical activation. This will require coding skills and training will be available for specific languages if required.

In addition to the development work, as part of the role you will be responsible for maintaining the MESMER website and dealing with questions from users. You will be responsible for promoting the use of MESMER.
The experimental and theoretical approaches will provide a very detailed understanding of the molecular mechanisms of chemical activation and energy transfer, however, it is also important to be able to include this new information into the current models that are used to model complex chemical systems. You will work with our partners to find ways to realistically and practically incorporate our understanding of chemical activation into practical models.

In addition to the master equation and modelling work that are the main priorities of the role, there will be potential to work in other areas of theory (ab initio calculations, molecular dynamics packages) or to contribute to some of the experimental work.

**What does the role entail?**

As a Research Fellow, your main duties will include:

- Working with experimentalists in interpreting results and developing understanding of chemical activation and energy transfer;
- Developing functionality in MESMER to better model chemical activation;
- Incorporating experimental and MESMER output into practical models of complex chemical processes;
- Maintaining the MESMER package and associated website;
- 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 work;
- Preparing papers for publication in leading international journals and disseminating research results through other recognised forms of output;
- Working both independently and also as part of a larger team of researchers, engaging in knowledge-transfer activities where appropriate and feasible;
- 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.

What will you bring to the role?

As a Research Fellow you will have:

- A PhD (or close to completion / or have submitted your thesis before taking up the role) in physical chemistry or a closely allied discipline;
- A strong background in computational chemistry, ideally including experience in modelling pressure dependent systems and in ab initio calculations;
- Expertise in programming;
- Good time management and planning skills, with the ability to meet tight deadlines, manage competing demands and work effectively under pressure without close support;
- A proven track record of peer-reviewed publications in high impact factor journals;
- Excellent written and verbal communication skills including presentation skills;
- A proven ability to work well both individually and in a team;
- A strong commitment to your own continuous professional development.

You may also have:

- Experience of pursuing external funding to support research;
- Experience in a wider range of computational chemistry, for example molecular dynamics or modelling complex systems;
- Experience of experimental work in gas phase kinetics or dynamics.

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:
Paul Seakins, Professor  
Tel: +44 (0)113 343 6568  
Email: P.W.Seakins@leeds.ac.uk

**Additional information**

**Faculty and School Information**
Further information is available on the research and teaching activities of the [School of Chemistry](#).

**A diverse workforce**
The Schools in the Faculty of Engineering & Physical Sciences are proud to have been awarded the Athena SWAN [Bronze or 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.

**Working at Leeds**
Find out more about the benefits of working at the University and what it is like to live and work in the Leeds area on our [Working at Leeds](#) information page.

**Candidates with disabilities**
Information for candidates with disabilities, impairments or health conditions, including requesting alternative formats, can be found on our [Accessibility](#) information page or by getting in touch with us at [disclosure@leeds.ac.uk](mailto:disclosure@leeds.ac.uk).

**Please note:** If you are not a British or Irish citizen, from 1 January 2021 you will require permission to work in the UK. This will normally be in the form of a visa but, if you are an EEA/Swiss citizen and resident in the UK before 31 December 2020, this may be your passport or status under the EU Settlement Scheme.

**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.