UNIVERSITY OF LEEDS

CANDIDATE BRIEF

Research Fellow in Computational Modelling of the Sorption Chemistry of Pollutants in Soils, Faculty of Environment

Salary: Grade 7 (£35,333 – £42,155 p.a.) This role cannot be appointed above £38,592 p.a. due to funding restrictions.

Reference: ENVFS1059

Fixed-term for 7 months, available immediately

Research Fellow in Computational Modelling of the Sorption Chemistry of Veterinary Antibiotics in Soils, School of Food Science and Nutrition, Faculty of Environment

Are you eager to work on processes underlying the environmental development of antimicrobial resistance? Are you interested in understanding the interactions of veterinary antibiotics with soil minerals? Do you have skills in first principles computational modelling?

This is an opportunity to work on a NERC Exploring the Frontiers pilot project looking at the sorption properties of mixtures of veterinary antibiotics and their metabolites on the minerals that make up the structure of agricultural soils. You will use the first principles DFT code, CASTEP, to run dynamic simulations of antibiotic sorption on kaolinite and goethite surfaces. This will provide an atomic-scale understanding of how these ubiquitous environmental pollutants interact with representative mineral components of soils and, critically, how competition between different antibiotics can lead to the retention of some antibiotics in the soil, and the wash-out of others into nearby water bodies. This is critically important with respect to the potential development of antimicrobial resistance (AMR) in the environment as well as the direct uptake of contaminants by lower animals and plants and their transfer into the human food chain. The project links to other research at the University of Leeds in this area, which will provide plenty of scientific interactions with other researchers.

You will have a background in theoretical/computational chemistry and an interest in the environmental fate of organic contaminants. Knowledge of CASTEP, or other first principles modelling software, would be an advantage.

What does the role entail?

As a Research Fellow, your main duties will include:

- Creating atomic-scale models of representative soil minerals, and veterinary antibiotics and their metabolites;
- Running multiple simulations using the first principles DFT code, CASTEP, to explore how these molecules interact with different mineral surfaces;
- Generating and pursuing independent and original research ideas within the scope of the project and beyond;



- Developing research objectives and contributing to setting the direction of the research project and team;
- Preparing papers for publication in leading international journals and disseminating research results through seminars and conferences;
- 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;
- 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 have submitted your final thesis before taking up the role) in computational chemistry or a closely allied discipline (theoretical physics; environmental or water chemistry; geosciences);
- A strong background in inorganic, organic or environmental chemistry;
- Knowledge of first principles or molecular dynamics simulation methods, preferably CASTEP;
- Experience of using high performance computing resources or a willingness to quickly learn these new skills;
- Good time management and planning skills, with the ability to meet tight deadlines, manage competing demands and work effectively under pressure without close supervision;
- A proven track record of peer-reviewed publications commensurate with career stage;
- 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;



- Knowledge or experience of environmental management of pollutants, enivronmental chemistry, mineral physics or pharmaceutical science.

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 Helen Chappell, University Lecturer
Email: h.f.chappell@leeds.ac.uk

Dr Laura Carter, Associate Professor
Email: l.j.carter@leeds.ac.uk

Additional information

Find out more about the Faculty of Environment.

Find out more about the School of Food Science and Nutrition

A diverse workforce
The Faculty of Environment is 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.

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.

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.