



UNIVERSITY OF LEEDS

CANDIDATE BRIEF

Research Fellow in Computational Chemistry for Repair of Tooth Enamel, School of Food Science and Nutrition, Faculty of Environment



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

Reference: ENVFS1163

Fixed-term for 12 months available from 1st October, 2026 to complete specific time limited work

We are open to discussing flexible working arrangements

Research Fellow in Computational Chemistry for Repair of Tooth Enamel, School of Food Science and Nutrition

Are you an ambitious researcher looking for your next challenge with a computational, industry-focussed project? Do you have a PhD in chemistry, physics, biology or materials science? Do you want to further your career in one of the UK's leading research-intensive Universities?

The Computational Chemistry, Biomaterials and Interfaces Group is based in the School of Food Science and Nutrition and works in an interdisciplinary way to investigate the fundamental science of biological systems.

We are looking for a Research Fellow to join a major project, funded by the BBSRC, STFC and Haleon plc: 'Building Molecular Simulation Capability for Digital Oral Care R&D as a First Step Toward an Artificial Mouth'. This project is led by Dr Helen Chappell within the School of Food Science and Nutrition at the University of Leeds. This position will be based full-time in Leeds but will work closely with project partners at Haleon and the STFC Daresbury Laboratory.

The post-holder will work on developing and testing a computational pipeline for assessing new ingredients for inclusion in dental consumer health products, e.g. toothpaste. The simulations will utilize molecular dynamics and first principles DFT codes to model enamel surfaces and their interactions with the environment of the mouth.

You will have experience of using molecular dynamics and/or density functional theory methods and a proven ability to structure, manage and work with quantitative data. You will be able to evidence designing and undertaking research, and contributing to a wider research programme; with experience of building working relationships with others from different backgrounds;

Main duties and responsibilities

- Running computational simulations using advanced research techniques (MD and DFT);
- Generating and pursuing original research ideas in the appropriate subject area;



- Developing research objectives and contributing to setting the direction of the research project with colleagues;
- Presenting findings of research, for example, preparing papers, blog posts and making presentations, with guidance and advice as appropriate;
- Preparing papers for publication in leading international journals and independently writing reports;
- Working both independently and as part of a larger team of researchers, and engaging in knowledge-transfer activities where appropriate and feasible;
- Maintaining your own continuing professional development and acting as a mentor to less experienced colleagues (e.g. undergraduate project students);
- Facilitating communications between collaborators by setting up meetings and sharing materials;
- Contributing to a positive research culture in the School;
- 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.

The post is based at the University of Leeds, on the main campus.

Qualifications and Skills

Essential

- A PhD (or near completion, i.e. the initial thesis needs to have been handed in at the point of application) in Physics, Chemistry, Materials Science or a closely allied discipline;
- Experience of using molecular dynamics and/or density functional theory methods.
- Proven ability to structure, manage and work with quantitative data;
- Evidence of designing and undertaking research, and contributing to a wider research programme;
- Experience of building working relationships with others from different backgrounds;
- Proven ability to write to the standard required for research reports/international publications;



- Good time management and planning skills, with the ability to meet tight deadlines and work effectively under pressure;
- Excellent written and verbal communication skills including presentation skills and the ability to communicate effectively with a wide range of stakeholders;
- Proven ability to manage competing demands effectively, responsibly, and without close supervision;
- A proven ability to work well both individually and in a team;
- A strong commitment to your own continuous professional development.

Desirable

- Expertise in using the DL_POLY or GROMACS molecular dynamics codes.
- A track record of high-quality publications that include some element of computational simulation;
- Experience of working with external stakeholders from industry or the public sector;
- Previous broad scholarly experiences, for instance, contributions to publications, individual and collaborative research projects, research proposals and applications for funding.

Additional information

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.

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: www.gov.uk/skilled-worker-visa

For research and academic posts, we will consider eligibility under the Global Talent visa. For more information please visit: <https://www.gov.uk/global-talent>

Find out more about the [School of Food Science and Nutrition](#).

Find out more about [Dr Helen Chappell](#).

Find out more about [Athena Swan](#) in the Faculty.



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.

Our University

As an international research-intensive university, we welcome students and staff from all walks of life. We foster an inclusive environment where all can flourish and prosper, and we are proud of our strong commitment to student education. Within the School of Food Science & Nutrition 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, those who belong to a minority ethnic community; people who identify as LGBT+; and disabled people. Candidates will always be selected based on merit and ability.

The Faculty of Environment has received a prestigious Athena SWAN silver award from [Advance HE](#), the national body that promotes equality in the higher education sector. This award represents the combined efforts of all schools in the Faculty and shows the positive actions we have taken to ensure that our policies, processes and ethos all promote an equal and inclusive environment for work and study.

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](mailto:hr@leeds.ac.uk).

Criminal record information

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.

