



UNIVERSITY OF LEEDS

CANDIDATE BRIEF

**Research Fellow in Electronic Structure Modelling,
Faculty of Engineering & Physical Sciences**



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

Reporting to Dr Andrew Scott

Reference: EPSPE1130

Fixed-term for 5 months, or 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 Electronic Structure Modelling

School of Chemical and Process Engineering

Would you like to work on the fundamental mechanisms of triboelectrification at the atomic and molecular scales using Density Functional Theory to elucidate the underlying triboelectric charge transfer mechanisms? Do you have experience in *ab-initio* electronic structure modelling using Density Functional Theory to understand and predict materials properties? Are you interested in working in a multidisciplinary team proactively tackling technical tasks in parallel?

Electrostatic charge accumulation in powders and grains, due to collisional and sliding contacts of surfaces of solids, commonly known as triboelectrification, is a nuisance and source of hazards, and at the same time, it has great potential for exploitation, as in the fast-growing technology of Tribo-Electric Nano-Generators (TENG). The former adversely affects manufacturability, due to issues such as downtime, valuable product loss and negative environmental impact, whilst for the latter, the identification of durable and efficient functional materials is highly desirable. The capability to predict triboelectrification tendency of materials provides a great competitive edge in advanced manufacturing across a wide range of industries from food and pharmaceuticals to additive manufacturing, polymers and TENG.

What does the role entail?

Using Density Functional Theory (DFT) and general molecular modelling methods, to study a number of materials of interest, ranging from model crystals to pharmaceutical crystals and polymers, relevant to our Industrial Partners. With your proven track record in this field, you will analyse and predict the nature of triboelectric charging by an electronic structure approach. Having experience in molecular visualisation and *ab-initio* (electron level) modelling, you will investigate molecular surface termination and electronic properties accountable for charge transfer. Our interest is in crystalline materials as well as from amorphous solid-state structures and in the effects of adsorbed water (due to relative humidity), charge modifying/neutralising chemical agents, and hydrophobic-hydrophilic contacts. Identification of materials functional groups accountable for maximum charge transfer is of interest for both TENG and charge mitigation in powders and grains. You will use the predictive capability to



interact with other activities in the programme and collaborate with our international teams and Industrial partners for verification and validation of simulations.

As a Research Fellow, your main duties will include:

- Using DFT methods (CASTEP or other suitable codes) to understand and predict charge transfer in a range of materials types;
- Building and visualising complex structures and surfaces;
- Using molecular mechanics force field methods to carry out molecular geometry optimisations prior to the more demanding DFT calculations;
- Using the high-performance computing (HPC) at the University of Leeds to enable the study of large, complex systems;
- Establishing a methodology for predicting the effective work function of facets of crystals, polymers, materials for TENG, functionalised glass beads, with and without anti-static agents;
- 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 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 have submitted your thesis before taking up the role) in *ab-initio* DFT modelling;
- A strong background in physical sciences or engineering and a deep understanding and prediction of materials properties at the atomic scale;
- Good time management and planning skills, with the ability to meet tight deadlines and manage competing demands effectively without close support;
- A proven 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 individually and in a team;
- A strong commitment to your own continuous professional development.

You may also have:

- Experience in molecular mechanics modelling;
- Experience of pursuing external funding to support research;
- Experience in effective work function measurements;
- Experience in fundamentals of triboelectrification.

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 Andrew Scott, School of Chemical and Process Engineering](#)

Email: a.j.scott@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 Chemical and Process Engineering | University of Leeds](#)

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 [AdvanceHE](#). The [Athena Swan Charter](#) is a framework which is used across the globe to support and transform gender equality within higher education and research. 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](#).

