



Project Title

Atomistic and Coarse-Grained Simulations of Polymer Composites

A PhD studentship is available in the group of Professor Philip J. Camp, School of Chemistry, University of Edinburgh (<http://www.molsim.chem.ed.ac.uk>) and with co-supervision from Professor Ken Lewtas, The Falcon Project and Visiting Professor at the University of Edinburgh.

The studentship is fully funded for 42 months by the University of Edinburgh, the Falcon Project, and the Defence Equipment & Support (DE&S) section of the UK Ministry of Defence, and covers tuition fees and an annual stipend at the UKRI rate (for 2024-25 this is £19,237 per annum) for a candidate satisfying EPSRC residency criteria

<https://www.ukri.org/what-we-do/developing-people-and-skills/esrc/funding-for-postgraduate-training-and-development/eligibility-for-studentship-funding/>).

Project Summary

The project will involve performing large-scale molecular dynamics simulations of the interactions between polymers and other components in highly filled composite systems, such as rubber products or rocket propellants. Simulations of failure mechanisms such as the formation and extension of cavities in polymers under stress will also be carried out, and the results will be linked with thermal and mechanical properties such as the heat capacity, thermal conductivity, shear modulus, and glass-transition temperature. The simulations will complement experimental work carried out by Professor Lewtas, and will inform the development of polymer matrices for energetic materials by the Falcon Project and DE&S. There will also be collaborative and computational support from the STFC Hartree Centre. The work will consist of performing all-atom simulations, developing reliable coarse-grained force fields, and applying those force fields to large-scale simulations to be compared with experiments. There will be opportunities for interactions with external partners, leading to knowledge exchange and demonstrable real-world impact.

Suitable candidates must possess, or expect to obtain, a first or upper-second class undergraduate degree (or equivalent) in chemistry, physics, or chemical engineering. Essential qualities include strong numerical skills, knowledge of statistical mechanics and the properties of soft matter, and familiarity with a programming language such as C/C++, Fortran, or Python. Some prior experience or exposure to molecular simulation techniques is desirable. Other important attributes are good presentation and communication skills (written and oral).

References

The Falcon Project: <https://www.ukspacefacilities.stfc.ac.uk/Pages/Falcon-Project-Ltd,-Westcott.aspx>

Defence Equipment & Support: <https://des.mod.uk/>

STFC Hartree Centre: <https://www.hartree.stfc.ac.uk/>

How to apply

In the first instance, an initial application consisting of a cover letter and a CV should be directed to Professor Philip J. Camp, School of Chemistry, University of Edinburgh, David Brewster Road, Edinburgh EH9 3FJ, UK. Email: philip.camp@ed.ac.uk

The position will remain open until filled. A closing date may be added later.

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IMPORTANT

Before submitting your cover letter and CV, please complete the online [School of Chemistry Equality, Diversity and Inclusion Form, entry 2025-26](#).

The form will automatically generate a unique 'Response ID number' that you must include in your cover letter.

Equality and Diversity

The School of Chemistry holds a Silver Athena SWAN award in recognition of our commitment to advance gender equality in higher education. The University is a member of the Race Equality Charter and is a Stonewall Scotland Diversity Champion, actively promoting LGBT equality.

The University has a range of initiatives to support a family friendly working environment.

For further information, please see our University Initiatives website:

<https://equality-diversity.ed.ac.uk/inclusion/family-and-carer>