



**PhD studentship (42 months):** Computer simulations of polymer additives in lubricants

**Academic Supervisor:** Professor Philip J. Camp, School of Chemistry, University of Edinburgh

**Industrial Supervisor:** Dr Beatrice N. Cattoz and Professor Peter J. Dowding, Infineum UK Ltd

A 42-month, industrially funded PhD studentship is available in the School of Chemistry at the University of Edinburgh under the supervision of Professor Philip J. Camp, Dr Beatrice N. Cattoz, and Professor Peter J. Dowding. The project will involve atomistic molecular-dynamics simulations of lubricants in the bulk-liquid phase and at liquid-solid interfaces under quiescent and shear conditions. The particular focus is on the conformations, association, adsorption, and tribological properties of polymer additives in oil-based lubricants. Molecular-dynamics simulations will be used to calculate structural and dynamical properties to complement tribological and neutron/X-ray scattering/reflectivity experiments coordinated by Infineum. The student will work within an Infineum consortium involving four other UK universities, Diamond Light Source, and Rutherford Appleton Laboratory. It will incorporate on-site training at Infineum, and the opportunity for participation in experiments at central facilities. Some relevant publications from recent work with Infineum are as follows.

1. 'Molecular adsorption, self-assembly, and friction in lubricants', R. F. G. Apóstolo, G. Tsagkaropoulou, and P. J. Camp, *J. Mol. Liq.* **277**, 606-612 (2019). <https://doi.org/10.1016/j.molliq.2018.12.099>
2. 'Effect of functional-group distribution on the structure of a polymer in non-aqueous solvent', R. F. G. Apóstolo, P. J. Camp, B. N. Cattoz, P. J. Dowding, and A. D. Schwarz, *Molecular Physics* **116**, 2942-2953 (2018). <https://doi.org/10.1080/00268976.2018.1511866>
3. 'Self-assembly and friction of glycerol monooleate and its hydrolysis products in bulk and confined non-aqueous solvents', J. L. Bradley-Shaw, P. J. Camp, P. J. Dowding, and K. Lewtas, *Physical Chemistry Chemical Physics* **20**, 17648-17657 (2018). <https://doi.org/10.1039/c8cp01785a>
4. 'Molecular Dynamics Simulations of Glycerol Monooleate Confined Between Mica Surfaces', J. L. Bradley-Shaw, P. J. Camp, P. J. Dowding, and K. Lewtas, *Langmuir* **32**, 7707-7718 (2016). <https://doi.org/10.1021/acs.langmuir.6b00091>
5. 'Glycerol Monooleate Reverse Micelles in Nonpolar Solvents: Computer Simulations and Small-Angle Neutron Scattering', J. L. Bradley-Shaw, P. J. Camp, P. J. Dowding, and K. Lewtas, *J. Phys. Chem. B.* **119**, 4321-4331 (2015). <https://doi.org/10.1021/acs.jpcc.5b00213>

A full description of the Edinburgh group's activities is given here: <http://www.molsim.chem.ed.ac.uk/>

The studentship is fully funded for 42 months from September 2019 or as soon as possible thereafter, and covers tuition fees and an annual stipend of £15,009 per annum for a candidate who satisfies the criteria for 'home' fees as defined here: <https://goo.gl/AtPII3>

The successful candidate will possess, or expect to obtain, a first or upper-second class undergraduate degree (or equivalent) in chemistry, physics, or chemical engineering. Essential qualities include basic knowledge of statistical mechanics and the properties of soft condensed matter, and familiarity with a programming language such as C/C++, Fortran, or Python. Some prior experience or exposure to molecular-simulation techniques and an interest in GPU computing are desirable. Other essential attributes are good presentation and communication skills (written and oral). In the first instance, informal enquiries (accompanied by a CV) should be directed to:

Professor Philip J. Camp

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Formal applications are made through the University's EUCLID system, as outlined here:

<http://www.chem.ed.ac.uk/studying/phd/applications-and-entry-requirements>

The position will remain open until filled.

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. See our University Initiatives website for further information. University Initiatives website: <https://www.ed.ac.uk/equality-diversity/help-advice/family-friendly>.