

UNIVERSITY COLLEGE LONDON

Job Description

Job Title:	Research Associate in Computational Chemistry
Department:	Institute for Materials Discovery / Department of Chemistry
Location:	UCL Bloomsbury Campus
Reports to	Dr Tung Chun Lee, Dr David O. Scanlon
Grade:	7

The Project

This position is available to work on the theoretical study of chemical reaction mechanisms in supramolecular systems. Detailed quantum mechanical (QM) simulations of potential intermediates and transition states can provide significant insight into the fundamental reaction mechanisms. These insights can then provide valuable context to experimental work, including facile study of analogous systems or derivatives. In combination with advanced mass spectrometry measurements, this project aims to explore anomalous chemical reactivity of organic molecules encapsulated within a molecular container. For instance, it is known that the reaction rate of a specific pathway can be enhanced if the intermediate species are stabilised by interaction with the cavity wall. Success of the project will reveal fundamental insights into how molecules react under nano-confinement that can lead to more efficient chemical processes and beyond.

This position is funded by the Leverhulme Trust for 12 months in the first instance. The candidate will join Dr Lee's and Dr Scanlon's research groups in the Institute for Materials Discovery and the Department of Chemistry at the Bloomsbury Campus of University College London. Information about the groups can be found on the group webpages: <http://tungchunlee.weebly.com/> and <http://davidscanlon.com/>.

Main Purpose

The post-holder will be required to carry out computational chemistry research into the reaction pathways of multiple reactive molecules within a molecular container. QM calculations will be performed using hybrid density functional theory, with the possibility for higher level methods. Identification and selection of promising host-guest pairs will be performed using QSAR models on large chemical databases. Further work will include investigation of functionalisation of both the host and the guest molecules. Computational work will be performed in collaboration with experimental efforts, and so the post-holder will also present results and contribute significantly to an interdisciplinary feedback loop.

Duties and Responsibilities

- To contribute to the selection and design of a series of guest molecules that exhibit rich and interesting chemistry, in collaboration with experimental chemists and other collaborators.
- To computationally investigate reaction mechanism pathways and perform transition state searching in a variety of host-guest complexes.
- To identify promising host-guest pairs using QSAR or other similar models on large chemical databases.

- To record, analyse and write up the results of the research in collaboration with a team of varied backgrounds.
- To contribute to the drafting and submitting of papers to peer reviewed journals.
- To contribute to the organisation of and to participate in mutual visits between project collaborators.
- To prepare progress reports on research for funding bodies as required.
- To contribute to the preparation and drafting of research bids and proposals.
- To contribute to the overall activities of the research team and department as required.
- To undertake a limited amount of teaching in relation to subject area.
- To contribute to the induction and direction of other research staff and students as requested.
- Responsible for ensuring that equipment is safe and maintained in working order.
- The job description reflects the present requirements of the post, and as duties and responsibilities change/develop, the job description will be reviewed and be subject to amendment in consultation with the post-holder.
- The post-holder will carry out any other duties as are within the scope, spirit and purpose of the job as requested by the line manager.
- The post-holder will actively follow UCL policies including Equal Opportunities and be expected to give consideration within their role as to how they can actively advance equality of opportunity and good relations between people who share a relevant protected characteristic and people who do not share it.
- The post-holder will maintain an awareness and observation of Fire and Health & Safety Regulations.
- To be aware of and act upon:
 - Disciplinary procedure and Disciplinary rules
 - Grievance procedure
 - Section 7 and 8 of the Health and Safety at Work Act

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Institute for Materials Discovery / Department of Chemistry

Person Specification for the Post of Research Associate

Knowledge – including Qualifications

PhD in Computational Organic / Materials Chemistry or a related discipline **[essential]**

Expertise in Computational analysis of reaction mechanisms and transition state searching **[essential]**

Knowledge of Physical Organic / Supramolecular Chemistry **[desirable]**

GCSE English Grade C or above (or equivalent, e.g. IELTS) **[essential]**

Skills

Proven research skills in computational chemistry, particularly QM and hybrid density functional theory **[essential]**

Ability to analyse and write up data **[essential]**

Ability to present complex information effectively to a range of audiences **[essential]**

Effective written and verbal communication skills **[essential]**

Experience

Experience of working in a research environment **[essential]**

Experience in performing interdisciplinary research **[desirable]**

Experience with the following: Gaussian or equivalent molecular QM code, Periodic DFT, Hybrid Density Functional Theory **[essential]**

Experience in using QSAR code and data mining **[essential]**

Experience in UNIX and LaTeX **[desirable]**

Experience of working with High-Performance Computing platforms **[desirable]**

Experience of interacting with experimentalists **[essential]**

Experience in supervising students **[desirable]**

Personal Qualities

Commitment to high quality research **[essential]**

Ability to work collaboratively and as part of a team **[essential]**

General Information

Terms & Conditions of Employment

The post is a UCL grade 7 post, the salary for which ranges from £34,635 to £41,864 per annum (including London Allowance of £3,031 p.a.). Starting salary is usually £34,635 per annum.

Please note, appointment at Grade 7 is dependent upon having been awarded a PhD; if this is not the case, initial appointment will be at Research Assistant Grade 6B (salary £30,316 - £31,967 p.a. inclusive of London Allowance of £3,031 p.a.) with payment at Grade 7 being backdated to the date of final submission (including corrections) of the PhD thesis.

Progression through the salary scale is incremental. Cost of living pay awards are negotiated nationally and are normally effective from 1st August each year. UCL's non-clinical pay and grading structure is at http://www.ucl.ac.uk/hr/salary_scales/final_grades.php.

UCL's terms & conditions for research staff are at

http://www.ucl.ac.uk/hr/salary_scales/Support_Research_tcs.php

The full range of benefits is at http://www.ucl.ac.uk/hr/benefits/employee_benefits.php

Equal Opportunities

UCL recognises that in our society, individuals and groups are discriminated against both directly and indirectly on the grounds of: age, colour, disability, ethnic origin, gender, HIV status, marital, social or economic status, nationality, race, religious beliefs, and responsibility for dependents, sexual orientation, trades union membership or unrelated criminal convictions.

To counteract discrimination, UCL is committed to actively opposing all forms of discrimination, raising awareness and tackling the causes and consequences. It is committed to providing a learning and working environment in which the rights and dignity of all its members are respected and which is free from discrimination, prejudice, intimidation and all forms of harassment including bullying; to making staff and students feel valued, motivated and enabled to do their best work and to creating a safe, welcoming working environment accessible to all.

The Department has been awarded a Bronze Athena Swan Award and we support the Athena beliefs that:

- The advancement of science, engineering and technology (SET) is fundamental to quality of life across the globe.
- It is vitally important that women are adequately represented in what has traditionally been, and is still, a male-dominated area.
- Science cannot reach its full potential unless it can benefit from the talents of the whole population, and until women and men can benefit equally from the opportunities it affords.

Further information on Athena Swan is at <http://www.athenaswan.org.uk/>

TO APPLY

Apply online at: <http://www.ucl.ac.uk/hr/jobs/> under **Ref no: 1671173**

You will need to register to use the system if you have not used it before and are able to do this after you have clicked on the '**Apply now**' button at the bottom of the page.

Thank you for your interest in this post and the Department of Chemistry at UCL